

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

Volume 16 · Issue 3

Collected archival edition

Original article text and available illustrations

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LETTER FROM THE PRESIDENT

Letter from the President



Sine Larsen

When I returned from the magnificent IUCr Congress in Florence after nine years on the Executive Committee as General Secretary and Treasurer, I had not imagined that I should become a member of the Executive Committee again and this time as the Chair of the Committee. It is a great honour for me to be elected President of the IUCr for the next triennium by the General Assembly and I shall do my very best along with the other members of the Executive Committee to further advance science and education in crystallography.

The IUCr was established in 1948 and is now 60 years old. In Japan the 60th birthday marks a significant point in life. It was therefore very appropriate to have the 60 years celebrations at the Congress in Japan. Many of the past IUCr Presidents contributed to the memorable anniversary celebrations: Ted Baker by an inspiring anniversary lecture illustrating the impact of crystallography, Andre Authier, Philip Coppens, Theo Hahn and Henk Schenk by open forum lectures to the public and young students, and last but not least, Bill Duax with a magnificent photo exhibition. I would like to take this opportunity to thank them warmly for all the work and dedication they put into their excellent contributions.

Publication of an international crystallographic journal was the driving force behind the creation of the Union, and this year *Acta Crystallographica* can also celebrate its 60th anniversary by the publication of the special issue *Crystallography across the Sciences 2*. *Acta Crystallographica* has developed into six specialized journals A to F, supplemented by *Journal of Applied Crystallography* and *Journal of Synchrotron Radiation*. The excellent staff in the Chester office has ensured the leading position of the Union among the scientific publishers. Their expertise in electronic publishing has been essential for the production of an electronic version of the International Tables. The publication of journals and books remains a core activity of the Union and keeping this activity at the forefront is one of the important tasks of the Executive Committee.

The growth of the journals reflects the growth of the IUCr. When the Union was formed in 1948 it had four founding Adhering Bodies representing four countries, now the IUCr has 40 Adhering Bodies representing 50 countries. A similar growth that reflects the impact of crystallography on many different scientific areas can be seen in the evolution of the number of Commissions. With the approval of the formation of the Commission on Crystallography in Art and Cultural Heritage at the Osaka Congress, this number has reached twenty compared to 1948, when there were six IUCr Commissions.

The work of the Union is directed by the General Assembly composed of the delegates from the Adhering Bodies as described by the Statutes and By-Laws of the Union. When one reads the Statutes and By-Laws it is clear that a lot of consideration was put into them by the founding fathers and mothers of the Union to protect the international nature of the Union and to ensure that developments of the Union are driven by science and not by national interests. The Statutes and By-Laws were last amended in 1999 to make them gender neutral.

In view of the evolution of the now 60 years old IUCr and the discussions that took place at the General Assembly in Osaka, it may now be timely to have a closer look at the Statutes and By-Laws. It was

agreed at the first meeting of the new Executive Committee to establish a special committee for this purpose, so possible changes could be ready for approval at the next General Assembly in Madrid.

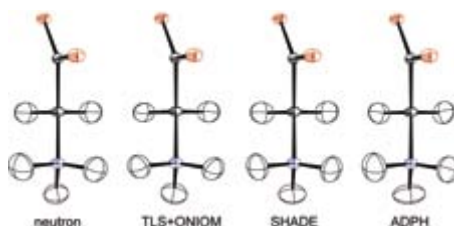
Sine Larsen

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IUCR JOURNALS NEWS

Estimated H-atom anisotropic displacement parameters: a comparison between different methods and with neutron diffraction results

Acta Cryst. (2008). A64, 465-475 (doi.org/10.1107/S010876730801341X)



ORTEP comparison of estimated H-atom APDs with neutron diffraction results for α -glycine. X-ray charge-density studies are increasingly being used to obtain *quantitative* information about chemical bonding and properties of molecules in the solid state. Most of these studies rely on accurate estimation of H-atom anisotropic displacement parameters (ADPs). Comparison of three different estimation approaches with each other and with neutron diffraction results demonstrated that all approaches are capable of giving accurate H-atom ADPs. Several benchmark systems were used to revise the web server <http://shade.ki.ku.dk>, and the SHADE approach is recommended as a routine procedure.

Parthapratim Munshi, Anders Ø. Madsen, Mark A. Spackman, Sine Larsen and Riccardo Destro

IUCR JOURNALS NEWS

Conformational variability of molecules in different crystal environments: a database study

Acta Cryst. (2008). **B64**, 348–362 (doi.org/10.1107/S0108768108005442)



Ephedrine in CSD entries EPHDHP and FIMVAY (a co-crystal) showing conformational differences due to rotation of the methylamino group.

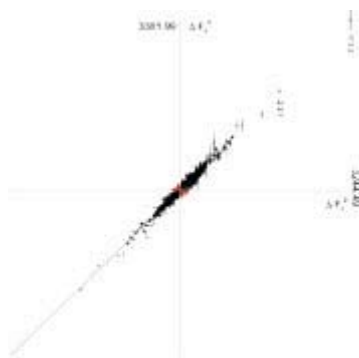
Are molecular conformations systematically affected by crystal environments? This study identifies organic molecules having multiple occurrences in the Cambridge Structural Database (CSD): alone, as solvates, co-crystals, *etc.* and uses cluster analysis to reveal their conformational variability. About 40% of flexible molecules adopt more than one conformation, but diversity arises principally through, *e.g.*, free rotation of functional group substituents, and in large-ring compounds, peptides, *etc.* – cases where different conformers are approximately equi-energetic. The study provides further reassurance that crystal conformations are good guides to conformational flexibility *in vacuo* and in solution.

Z. F. Weng, W. D. S. Motherwell, F. H. Allen and J. M. Cole

IUCR JOURNALS NEWS

Was Bijvoet right? Sodium rubidium (+)-tartrate tetrahydrate revisited

***Acta Cryst.* (2008) C64. m296-m299 (doi.org/10.1107/S0108270108022415)**



Plot of observed vs. calculated Bijvoet differences, prepared using the program PLATON. 842 reflections with the correct sign are shown in black, 92 reflections with the wrong sign in red.

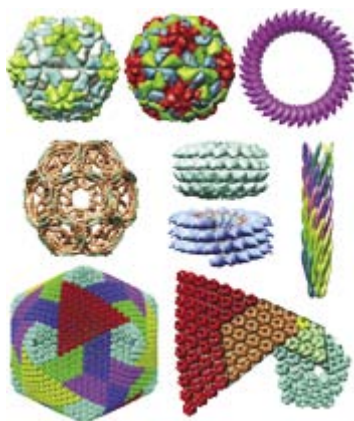
The first absolute structure determination of a chiral organic compound was performed on sodium rubidium (+)-tartrate by Bijvoet, Peerdeman and van Bommel in 1951. By repeating this experiment with recent equipment and methods, the absolute structure assignment *R,R'* for C2 and C3 was unequivocally confirmed in the present study. Flack parameter $x = -0.007(6)$; Hooft parameter $y = -0.011(4)$.

M. Lutz and A.M.M. Schreurs

IUCR JOURNALS NEWS

Representation of viruses in the remediated PDB archive

***Acta Cryst.* (2008). D64, 874-882 (doi.org/10.1107/S0907444908017393)**



A new scheme has been devised to represent viruses and other biological assemblies with regular noncrystallographic symmetry in the Protein Data Bank (PDB). The scheme uses generalized descriptions of deposited and experimental coordinate frames, symmetry and frame transformations. A simple notation encodes the generation of assemblies from deposited coordinates and matrix operations. Complete correct information for building full assemblies, subassemblies and crystal asymmetric units of all virus entries is now available in the remediated PDB archive.

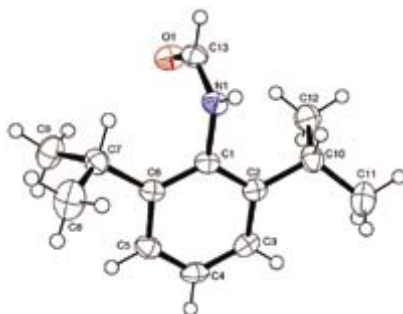
*C.L. Lawson, S. Dutta, J.D. Westbrook, K. Henrick and
H.M. Berman*

IUCR JOURNALS NEWS

N-(2,6-Diisopropylphenyl)formamide

N-(2,6-Diisopropylphenyl)formamide

Acta Cryst. (2008). E64, o1728 (doi.org/10.1107/S1600536808024811)



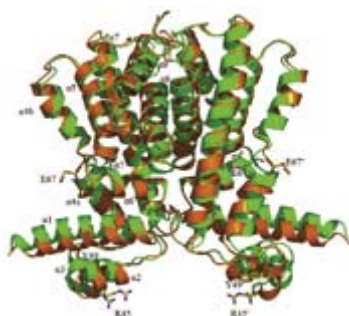
N-(2,6-Diisopropylphenyl)formamide exists as two carbon–nitrogen bond rotomers in solution. Upon crystallization, however, the solid-state structure shows exclusive formation of the *cisoidal* rotomer. The compound exhibits a non-planar structure in which the 2,6-diisopropylphenyl ring is tilted at a dihedral angle of 77.4(1)° with respect to the formamide moiety. This is the largest dihedral angle known among structurally characterized formamides and is attributed to the presence of the bulky isopropyl groups on the *ortho* positions of the phenyl ring, which increases torsional strain between the two planes defining the dihedral angle.

J.M. Chitanda, J.W. Quail and S.R. Foley

IUCR JOURNALS NEWS

Conformational change of the AcrR regulator reveals a possible mechanism of induction

***Acta Cryst.* (2008). F64, 584-588 (doi.org/10.1107/S1744309108016035)**



Structural comparison of the $P3_1$ and $P222_1$ structures of AcrR.

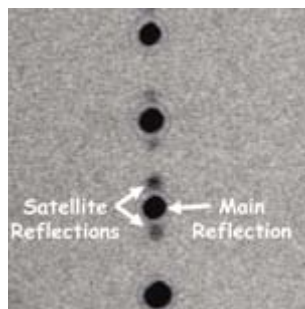
Escherichia coli AcrR represses transcription of *acrAB* and is induced by many structurally unrelated cytotoxic compounds. The crystal structure of this regulator in space group $P222_1$ has been reported previously, revealing a dimeric two-domain molecule with an entirely helical architecture similar to members of the TetR family of transcriptional regulators. Here, a crystal structure of this regulator in space group $P3_1$ is presented. A comparison of the two AcrR structures reveals possible mechanisms of ligand binding and AcrR regulation.

R. Gu, M. Li, C.-C. Su, F. Long, M.D. Routh, F. Yang, G. McDermott and E.W. Yu

IUCR JOURNALS NEWS

Protein crystals can be incommensurately modulated

J. Appl. Cryst. (2008). 41, 600–605 (doi.org/10.1107/S0021889808010716)



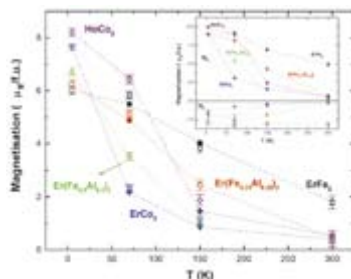
Incommensurately modulated PA crystal with main reflections indexed and predicted (blue circles) with space group $P222$, $a = 38.1$, $b = 72.3$, $c = 185.7$ Å and showing satellite reflections in one modulation direction indexed as $\mathbf{q} = 0.29\mathbf{b}^*$.

Modulated crystals result in diffraction patterns consisting of main reflections surrounded by satellite reflections. These patterns are typically encountered in small-molecule structures at the interface of a phase transition. If the modulation is incommensurate then the satellite reflections cannot be predicted with a supercell. In these cases a superspace indexing approach is used to index the reflections. We report a successful superspace indexing of an incommensurately modulated crystal of profilin:actin. In this case the modulation is induced with a pH change.

Jeffrey J. Lovelace, Cameron R. Murphy, Lee Daniels, Kartik Narayan, Clarence E. Schutt, Uno Lindberg, Christer Svensson and Gloria E.O. Borgstahl

Disentanglement of magnetic contributions in multi-component systems by using X-ray magnetic circular dichroism at a single absorption edge

J. Synchrotron Rad. (2008). **15**, 440–448 (doi.org/10.1107/S0909049508017652)



Comparison of the temperature dependence of the magnetisation measured by using a standard SQUID magnetometer and that derived from the magnetisation of the rare-earth and transition-metal sublattices determined from the rare-earth L_2 -edge XMCD spectra.

X-ray Magnetic Circular Dichroism (XMCD) has proved to be one of the most outstanding tools to study magnetism by incorporating the atomic-element specificity inherent to a core-level spectroscopy. XMCD is a simultaneous fingerprint of the magnetic contributions to the conduction band coming from the different elements in the material. Our approach provides a method of disentangling these contributions that opens the possibility of performing element-specific magnetometry by using a single X-ray absorption edge.

J. Chaboy, M.Á. Laguna-Marco, C. Piquer, R. Boada, H. Maruyama and N. Kawamura

IUCR ACTIVITIES

An Inspiring new Commission: CrysAC*



The members of the CrysAC Commission at the IUCr2008 Osaka meeting, during the first Open Meeting of the newly formed commission (courtesy of Prof. R. Gould, University of Edinburgh). From left to right: Abdelmalek Thalal, Alicja Rafalska-Lasocha, Simona Quartieri, Eric Dooryhée, Cele Abad-Zapatero, Anke Zürn, E. Makovicky (Gautam Desiraju is absent).

The relationship between Crystallography and Art, or more personally crystallographers and artistic expression, has always been very flirtatious based on an immediate attraction between the two partners. Crystallographers specially, but also earlier scientists like Leonardo and Kepler, are drawn naturally to the fascinating beauty of the structures and patterns that they unveil hidden in the crevices of their unit cells. The attraction seems irresistible!

With those images in our eyes, we might have soon discovered the work of the pioneer Viennese graphic artist Koloman Moser [1](1868-1918) or the work of the better known Dutch graphic artist (M.C. Escher: 1898-1972) and his imaginative excursions into the tiling of the plane; to him it was like an obsession. His color plates and those of others (H. Hinterreiter, 1902-1989) illustrated the concepts of polychromatic symmetry arguably before this notion appeared more widely in the literature. Moreover, Escher's later works used his amazing artistry and richness in detail to depict imaginary self-reflecting worlds that were braided together with Gödel and Bach in that imaginative, tripartite golden braid written by Douglas Hofstadter entitled *GEB (Godel, Escher, Bach)* inviting all of us to reflect upon the unique threads of the human spirit, upon our own consciousness and who we are.

It is well documented that Escher got his inspiration to explore the tiling of the plane from the ceramic tiles that he saw in the magnificent palace of the Alhambra in Spain in 1936 during one of his trips to Andalusia. If this was a window of inspiration for him, it is also a source of study, analysis and exploration for an enlarging group of crystallographers and mathematicians exploring geometric patterns in Islamic

art (see for instance www.castera.net). This field of study now encompasses Moorish *zillij* (tile) patterns including *taqshir* calligraphic patterns in the Alhambra and in many other places in the Islamic world: Blue Mosque in Istanbul, Kharragan tomb towers in Iran, decorations at *Mihrab*, (the inner sanctum of the Islamic Mosques), among others. The maturity of this field of study is evident by the existence of an IUCr commission devoted to these topics (MaThCryst: www.crystallography.fr/mathcryst) and the multitude of papers that continue to appear on these topics ranging from the description of the decorations, to the detailed mathematical analysis and to the understanding of the artisanal and practical aspects of these artistic manifestations of the human spirit. A significant review of the current work in the field was presented at the satellite meeting of the European Crystallographic Society (ECM24) in Marrakech entitled *The Enchanting Crystallography of Moroccan Ornaments*, sponsored by the MaThCryst commission.

The study of symmetrical patterns in other human artifacts across different cultures such as Javanese Batik cloths, Pueblo Indian Pottery, Japanese feudal emblems (i.e., *manji* and *kamon*), Oriental carpets, Indian floor patterns (*kolam*) and others is an active area of research. The scope of these investigations is enormous and detailed studies might unveil unknown cross-pollination and influences between the different cultures in space and time; or it could reveal independent discovery of symmetrical patterns of decorations and motifs by the human mind (see bibliographies at www.crystallography.fr/crysac/bibliography.php and below).

What else is there besides the mathematical theory of ornamentation to attract crystallographers to art? What can the experimental methods related to crystallography add to the understanding of the relationship between Art and Crystallography or even more encompassing Art and Science? As noted by C.P. Snow, the schism between the two cultures became more significant in the 19th century but there is great impetus to bring these two critical threads of the human spirit together again and crystallography could provide a unique bridge and agglutinant. There is a tremendous amount of academic research on this theme with Art historians, artists, scientists and cultural observers all over the world taking sides on a continuous spectrum with two separate poles. Can the relationship between Art and Science be described by the nebulous concept of 'spirit of the times' (as embedded in the German word '*Zeitgeist*'), or is there a real causal link between Art and Science supported by concrete evidence? A large number of books (the most famous being probably the Shubnikov & Koptsik text on *Symmetry in Science and Art*) and research papers published in professional journals by the leaders in the field (see full article on the IUCr website) who present their individual work or review that of others and address this question in various ways. The range of studies is enormous and details can be found on the commission's website or see www.leonardo.info/isast/spec.projects/artsciencebib.html for a non-exhaustive but annotated bibliography.

Crystallographic and related techniques (diffraction, spectroscopy, microanalysis and microimaging) applied to the microanalysis of samples (both crystalline and amorphous) originating from ancient paints, pottery, cosmetics, unguents, archaeological materials, preserving materials and many others can provide critical information on the composition, origin, production technology, authenticity, physical and cultural migration, historical development and other related issues. Thus, it can provide unambiguous evidence to Art scholars and historians, critics, archaeologists and anthropologists battling with questions that cannot be answered by more traditional methods. What branch of science or technology can claim such a wide range of 'artistic' leanings and applications with direct impact in the Art-Science interface?

In response to the growing interest and developments in the use of crystallographic methods to analyze historical, cultural and archaeological artifacts (among others) the Executive Committee of the IUCr at its meeting in Osaka (August 2008) approved the formation of a new commission appropriately named 'Crystallography, Art and Cultural Heritage (CrysAC)' devoted to the support and expansion of all of those lines of enquiry. The decision followed the request presented by E. Dooryh  e (CNRS, France) who has been the leading force behind a proposal drafted by a group of crystallographer colleagues

interested in this area of research [1]. The terms of governance, objectives and vision of this new commission as well as its current membership and group of supporting consultants can be found at www.crystallography.fr/crysac/. A satellite symposium organized jointly by the MaThCryst and CrysAC commissions will be held at the next meeting of the European Crystallographic Assn (ECM25) in Istanbul (Turkey, August 2009) devoted to the theme of *Symmetry and Crystallography in Turkish Art and Culture*. [2]

Any person interested in pursuing the scientific problems that this branch of crystallography is trying to address should always keep in mind three cardinal points as beacons to guide her or his interests in the areas of research that this commission seeks to explore at the interface of Art and Science. First, the analysis, explanations and insights into the artifacts/samples do not destroy the beauty and uniqueness of the objects under study no matter how aseptic the language of mineral names, textures, chemical formulae and space groups might sound. Second, the scientific and technological aspects represented and underlying in any form of Art (graphic, decorative, architectural or other) are a part of the cultural heritage of the societies and people of the Earth who created them. Finally, it is through the wise and intelligent usage of the findings, explanations and concepts expressed above that we can make our work and our discoveries more accessible to lay people so that the discoveries enrich their lives as much as they enrich ours; our findings can illuminate Art in unique ways for the specialist and for our fellow humans. We feel that the new commission created by the IUCr provides an inspiring opportunity to achieve all these goals in future years.

Visit the website of this new CrysAC commission of the IUCr (www.crystallography.fr/crysac/) or join the open mailing list at <http://listes.uhp-nancy.fr/www/info/crysac>. We welcome your comments, suggestions and insight as to the goals, objectives, directions and strategies of this new commission to make this new initiative of the IUCr a complete success for all of us and for society at large.

Cele Abad-Zapatero on behalf of the members of the Commission on Crystallography, Art and Cultural Heritage of the IUCr

*This is an abridged version of a full motivation essay that can be found at the commission's website (www.crystallography.fr/crysac/motivation.php).

Notes

[1] During the Microsymposium *Crystallography and Understanding of Cultural Heritage* chaired by H. Schenk and S. Siano (XX Congress of IUCr, 2005, Florence), the concept of a new IUCr commission emerged. Eric Dooryh  e, who presented a lecture – *Powder diffraction in art and archaeology* there and who had experience in the investigation of objects from art and archaeology, gave substance and body to the proposal with input from interested colleagues.

[2] www.crystallography.fr/mathcryst/istanbul2009.php

NOTICE

IUCr Support for National Meetings in Developing Countries

The scope of meetings that may be supported through the Sub-committee on the Union Calendar has been extended so that national meetings that are held in developing countries are now included. Such meetings will also be eligible for support through the Visiting Professorship scheme, where appropriate.

Organizers of national meetings in developing countries interested in applying for support for young scientists and/or Visiting Professorships should contact the Chair of the Sub-committee on the Union Calendar (Professor G.R. Desiraju: gautam_desiraju@yahoo.com) or the Executive Secretary (execsec@iucr.org) to request an application form.

(The IUCr Visiting Professorship Scheme will pay the travel and insurance costs for up to three eminent scientists to enable them to present a short course at a workshop or school. The local organizers cover the accommodation/subsistence expenses.)

MEETING REPORT

XXI Congress and General Assembly



IUCr2008

Osaka, Japan, August 23-31

www.iucr2008.jp/



Left: Tomitake Tsukihara, Chair of the Local Organizing Committee. Centre left: Yasuhiko Fujii, Japan, Chair of the International Program Committee. Centre right: David Sayre. Right: David Sayre receives 2008 Ewald Prize at Opening Ceremony.



Left: IUCr President Yujii Ohashi and Yukako Ohashi. Right: Newly elected IUCr President Sine Larsen and Henk Schenk



Left: The conference took place at the Grand Cube, Osaka. Right: Downtown Osaka.



Left: Entertainment at Opening Ceremony. Right: Photograph exhibit celebrating the 60th anniversary of the IUCr.

The XXI Congress and General Assembly of the International Union of Crystallography was held from August 23-31, 2008 at the Osaka International Convention Center (Grand Cube Osaka). The total number of participants, including guests was 2,617. Plenary lectures were presented by S. Iijima on carbon nanotubes and by K. Wuthrich on combining NMR and X-ray crystallography in post genomic biology. During the opening ceremonies E. N. Baker presented a plenary lecture in celebration of the 60th anniversary of IUCr in which he gave a beautiful overview of the history and wide range of applicability of crystallography. The 8th Ewald Prize was presented to D. Sayre for the unique breadth of his involvement in crystallography ranging from seminal contributions to the solving of the phase problem to the complex physics of imaging generic objects by X-ray diffraction and microscopy. Thirty-six speakers provided keynote lectures on leading-edge science in their respective fields. Seven parallel oral sessions were held each day, which stimulated useful discussions. Additionally, 1,500 posters were presented over six days; 500 posters were displayed at a time for a period of two days. There were 55 companies represented in the commercial exhibit in the poster area. The participants also enjoyed sightseeing and Japanese culture.

Tomitake Tsukihara

Keynote Lectures

Power to the proteins powder



Rena Margiolaki

Rena Margiolaki (ESRF, France) presented a summary of the emerging field of protein powder diffraction. She reviewed early work by Bob Von Dreele on Met myoglobin, a new structure of human insulin and complexes of hen egg white lysozyme with glucosamine oligomers. She described the feasibility of using powder diffraction to solve protein structures by molecular replacement and initial results obtaining molecular envelopes using heavy atom derivatives. She described phase changes observed during cryocooling, new insulin phases and the solution of a urate oxidase tetramer with more than 10,000 atoms by molecular replacement.

R. Von Dreele

Nanostructures on Surfaces



Cristian Mocuta

The physical properties of nanostructures differ from those of larger assemblies because large surface to volume ratios alter energetics and internal structure. In the past, X-ray beams were too large to probe single nanostructures, forcing interpretation of the scattering from averages of many nanostructures. Cristian Mocuta (ESRD, France) described how X-ray scattering studies using synchrotron radiation with beams sufficiently small to probe individual nanostructures are providing valuable new insights into these materials.

S. Gruner

Refinement and Modelling of Complex Mineral Structure (KN36)

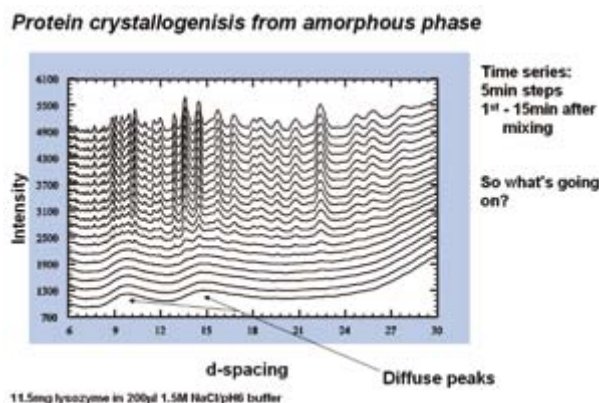


Roberta Oberti

Roberta Oberti (U of Pavia, Italy) demonstrated how complex mineral systems, like the amphiboles, with highly coupled multi-site, multi-species substitutions can be characterised. Their secrets can be unravelled by a combination of diffraction, spectroscopy and crystal-chemical modelling. The latter allows not only a deeper understanding of observed particularities, but also possesses predictive power, for instance with respect to the occurrence and distribution of species such as H, Li, Be or B which are otherwise barely detectable.

Wulf Depmeier

Lasers, Jet Streams, Turkish Spiders and Powder Power (MS09)



New technologies are becoming available to study micron-sized crystallites and multiple crystal clusters. Tiny crystallites can be studied one by one, as polycrystals or as powders. The formation of a nucleus of a crystal can also be studied by diffraction techniques. Bob von Dreele (USA) has monitored the transition from solution to amorphous to single micro crystals of lysozyme (Figure 1). New X-ray lasers may have sufficient photons per 10 fsec pulse to obtain diffraction patterns from a single protein molecule before radiation destroys the sample. Alternatively, if the photons per pulse are low, a 10x10x10 cluster of proteins may yield the necessary intensity statistics. David Shapiro (USA) showed the first ever protein powder diffraction from a stream of tiny crystallites of photosystem I (PSI) that were measured at the Hamburg FLASH Facility using gas jets and soft X-rays. The wavelength used did not lead to absorption with these 'micro-jet' sample thicknesses and the powder pattern had well resolved lines. Sebastian Basso (Switzerland) reported successful determination of protein envelopes and secondary structure features at ~4 Å resolution using MIR phasing at ESRF. Yoichiro Hosokawa (Japan) described the use of a fsec infra-red laser to either cut a fragment of a crystal from a cluster without thermal damage or to irradiate a solution with laser pulses to promote nucleation. The Session chair was startled to learn that the technique has been used to crystallize membrane proteins. Pinar Batat (Turkey) examined the silks from many varieties of Turkish spiders with electron microscopy, SWAXS, XRD and tensile strength measurements. Optimal structural properties were found in silk from well nourished spiders in quality habitats.

John R. Helliwell

Crystal Chiral Chemistry, New Ideas, New Instruments (MS14)

Crystallographic analysis allows the study of the chirality of a molecular assembly and its functionality. In this symposium a wide range of topics involving chirality were discussed, including growth conditions, properties, the computational chemistry of chiral crystals and their use in absolute asymmetric synthesis. Of particular interest was a description of the Universal Chiroptical Spectrophotometer (UCS), being built by R. Kuroda and co-workers (Japan) that will permit artifact-free CD measurements for crystalline powder samples.

Ichiro Hisaki

The Interface between CryoEM and Crystallography (MS22)



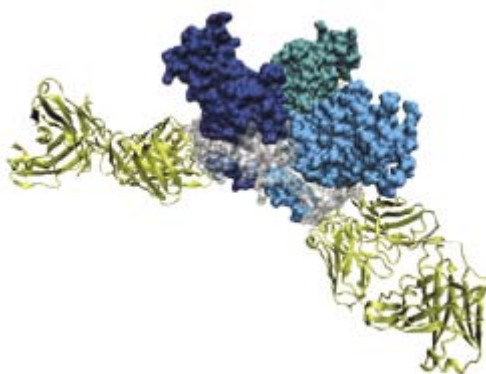
Session on the interface between CryoEM and Crystallography

In this microsymposium Steve Ludtke (Baylor College of Medicine) showed Electron Microscope (EM) reconstructions in which all main-chain secondary structure and many side-chain atoms were resolved, and a movie of domain movement in a fatty acid synthetase. Tom Blundell (UK) expressed surprise at how well a structure could be modelled into a 4 Angstrom resolution map. Steve noted that unlike crystallographic maps, CryoEM maps have very reliable phases and less-reliable amplitudes, so map errors are qualitatively different.

Structure determination of the epsilon15 virus by cryoEM (Wen Jiang, USA) required collection of 3000 images and 1 million cpu-hours to calculate the reconstruction (10 days per cycle on a supercomputer cluster). Ed Egelman (USA) presented structural results using his helical processing technique and observed that individual subunits in fibrous structures are highly conserved, but quaternary structure interactions between subunits diverge. Atsunori Oshima (Japan) described a gap junction in a 2-layer 2D crystal, and mutational analysis indicating that a plug at the entrance to the pore consists of N-terminal residues. Elizabeth Villa (USA) has a novel method to fit EM maps using restrained molecular dynamics. She showed a movie in which parts of a ribosomal structure move large distances to fit an EM map. The method will be available as a module of the program VMD. Cathy Lawson (USA) described deposition and archiving of EM maps at the EM databank (emdatabank.org)

Wah Chiu and Cathy Lawson

Virus Structure and Antiviral Strategies (MS29)



Structure of the Ebola virus glycoprotein PDBid = 3CSY in complex with a neutralizing antibody from a human survivor. The structure reveals a putative receptor-binding site sequestered in a bowl of the chalice formed by three GP1 subunits (colored in shades of blue), wrapped around by three GP2 fusion subunits (colored white). The antibody fragment (colored yellow) bridges the GP1 and GP2 subunits and is specific for the prefusion viral surface conformation of GP2. (J. E. Lee, M. L. Fusco, A. J. Hessel, W. B.

Oswald, D. R. Burton, and E. O. Saphire. (2008). *Structure of the Ebola virus glycoprotein bound to an antibody from a human survivor*. *Nature*, 454, 177-182.)

Crystal structures of medically and economically important viruses revealed how these smallest and simplest biological entities survive and replicate, fostering the development of strategies to prevent animal and human disease. Peter Kwong (USA) presented a structure of HIV gp120 complexed with a neutralizing antibody Fab fragment, which showed it only binds with heavy chain, and that HIV gp120, and perhaps HIV as a whole, only has one 'attack' point for neutralizing antibodies. The identified epitope has been disguised in a recombinant protein with the aim of using this protein as a vaccine. Nuria Verdaguer (Spain) presented structures of viral RNA-dependent RNA polymerases from birnavirus and foot and mouth disease virus with bound substrates. Felix Rey (France) also talked about birna viruses but focused on the capsid and evolutionary relationships, noting that picobirna viruses are not structurally related to birnaviruses.

The sole Ebola virus surface protein, GP, which is post-translationally cleaved to give GP1 and GP2, was described by Jeff Lee (USA). It was crystallized with a monoclonal antibody Fab fragment from a human survivor of the Kitwit Ebola outbreak in Zambia. Like HIV, gp120 is predicted to be almost entirely covered by glycosylation. Rolf Hilgenfeld (Germany) pointed out that all recently (re)-emerging viruses (avian influenza, SARS, Marburg, and others) are RNA viruses and advocated the need for studying all animal viruses, to be prepared for the emergence of human variants. If lead compounds can be developed against them, several years will have been gained when a virus does emerge. He presented structures of several RNA virus proteases and ongoing work to develop inhibitors for them. Funding for this will have to be at least partially public, as big pharma will not be financially interested.

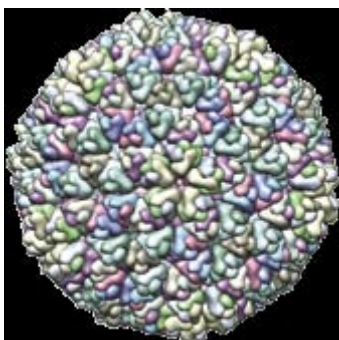
J. Johnson and M. J. van Raaij

Advanced Electron Microscopy (MS34)

This microsymposium highlighted applications and instrumental developments in electron microscopy with an emphasis on high resolution imaging in the Transmission and Scanning Transmission Electron Microscope (TEM and STEM). Kazuo Suenaga (Japan) presented spectacular images at close to atomic resolution of conformational changes in retinal molecules encapsulated within carbon nanotubes. Susanne Stemmer (USA) discussed possible origins of the 'Stobbs Factor' in Annular Dark Field STEM imaging and showed how careful experimental calibration of the detector response function and the use of a frozen phonon model for calculation of ADF intensity enabled quantitative imaging. Andrew Bleloch (UK) discussed recent work at the UK SuperSTEM facility showing the location of gold impurity atoms in silicon nanowires and the use of discrete tomography from a limited projection set of ADF images to determine morphology in metallic nanoparticles. Osamu Kamimura (Japan) described the development of a novel microscope, operating at 30kV, optimized for recording coherent electron diffraction patterns for use in phase retrieval/phase extension algorithms. Gianluigi Botton (Canada) provided an overview of the use of aberration corrected TEM and STEM imaging coupled to EELS in the study of catalysts and pyrochlore structures that show magnetic frustration.

A. I. Kirkland and R. Holmestad

MS36 Huge and Complex Viruses and Proteins



Assembly of rice dwarf virus PDBid = 1UF2. (Toshihiro Omura)

This symposium featured a fascinating animation of the assembly process of the rice dwarf virus (T. Omura, Japan). It is one of the largest viruses for which the three-dimensional structure has been determined. The architecture of a virus infecting archaea (A. Goulet, France) was shown to be different from most other known viruses. It resembles the organization found in nucleosomes. Other topics covered were reconstruction of ion channels using single particle analysis (Chikara Sato, Japan), the structure of the giant muscle protein titin (M. Wilmanns, Germany) and Holliday junction resolvases (D. Suck, Germany).

M. R. N. Murthy and K. Iwasaki

Charge Flipping and Relaxation in Real Space (MS62)

A microsymposium on real space direct methods focused on algorithmic advances. While nonconvexity of the various phase retrieval problems presented in the session remains a sensitive issue, new algorithms or variants of existing algorithms make it possible to achieve better convergence profiles and to avoid local minima. Specific topics included developing algorithms for recovering protein structure from signals with very low photon counts (D. Saldin, USA), alternating thresholding/projection algorithms in the spirit of charge flipping methods, forcing both the known magnitude data in reciprocal space and a degree of sparseness in real space (S. Marchesini, USA), projection/reflection relaxation schemes for phase retrieval in diffraction imaging (R. Luke, USA), algorithms for handling inverse problems via subgradient projection techniques (I. Yamada, USA), and a solution to the phase problem for surface X-ray imaging (I. P. Lyman, USA).

P. L. Combettes

Co-crystals: Theory, Synthesis and Use (MS66)

Describing 'Multi-component solids in crystal engineering', Gautam R. Desiraju (India) noted that early descriptions of multi-component molecular crystals pre-date the modern concept of crystal engineering. He described the introduction of reliable chemical information into engineered crystals with supramolecular synthons that permit discrimination between likely and less likely structural products and his visions of future directions within the fields of chemical crystallography and crystal engineering. Christer B. Aakeröy (USA), 'From a molecular dating agency to successful co-crystal synthesis', focused on co-crystal synthesis as an analogue of molecular synthesis, including 'supramolecular yield' and 'supramolecular selectivity'. He stressed that co-crystal chemistry should not be restricted to systems that prove to be amenable to single-crystal X-ray structural analysis and presented research utilising a diverse range of tunable, site-specific intermolecular interactions for programmed design of co-crystals containing two or three different molecular components, as well as larger supramolecular systems such as molecular capsules. William Jones (UK) illustrated a broad range of multi-component systems, with emphasis on pharmaceutical products. He showed that solvent-assisted mechanical grinding permits comprehensive screening of multi-component chemical systems and can yield co-crystals that are

different from those obtained using solution techniques. An example of efficacious co-crystallization is the improved stability of caffeine afforded by co-crystallization with oxalic acid.

Carol P. Brock (USA) presented a detailed analysis of a two-component molecular system, ordered layers of triphenylphosphine oxide with disordered layers of hydrogen-bonded cyclohexane dialcohol molecules. The system resisted a satisfactory solution until improved instrumentation became available for data collection. One particularly intriguing aspect of the study was an apparent relationship between the degree of order in the co-crystal and the solvent used for crystallization, which might go on to yield interesting information regarding the role of solvent intervention in the crystallization process. In a talk combining *in situ* co-crystallization with Raman spectroscopy, Michael Kirchner (Germany) described experimental procedures for co-crystallization of the smallest molecules that are usually liquid or gas under ambient conditions. Attempted crystallizations of these compounds yielded only microcrystalline products. The value of spectroscopic techniques was stressed for these cases to ascertain whether or not co-crystallization had actually occurred, and an *in situ* installation of a probe for Raman spectroscopy was highlighted. The session was complemented by a keynote lecture by Michael J. Zaworotko (USA) that provided further visions and examples for development in this active research area.

Maio Du and Andrew D. Bond

Diffuse Scattering in Partially Disordered Systems (MS77)

Richard Welberry (Australia) reviewed a wide-range of diffuse scattering phenomena in many different systems, and demonstrated the use of single-crystal X-ray diffuse scattering to extract local correlations in disordered molecular systems. Monte Carlo simulations employing inter- and intramolecular spring constants reproduced all of the key features in the experimental patterns. Miwako Takahashi (Japan) measured magnetic diffuse scattering at KENS in Pt-rich PtMn alloys (the new ABC6 structure) and identified diffuse incommensurate satellites with intermediate-range incommensurate spin-density waves induced by Fermi-surface nesting. Sonia Francoual (USA) identified diffuse-scattering signatures of phason diffuse scattering in X-ray patterns of icosahedral Zn-X-Sc (X = Co, Ag, Mg) quasicrystals, and successfully measured the phason elastic coefficients (for zero phason-phonon coupling) that were insightfully related to the electronic structure and composition and atomic radius of element X. Thomas Weber (Switzerland) demonstrated novel 3D PDF analysis techniques for extracting local structure information from quasicrystal diffuse scattering patterns. Clever data reduction strategies that isolate one type of feature at a time in Q-space greatly simplify the preparation and interpretation of the PDF. In photochromic cuprous-halide nanocrystals embedded in a glassy boro-alumino-silicate matrix, doped with Cd and Sn, Sylvio Haas (Germany) showed that the analysis of multi-resonant small-angle X-ray scattering data can recover complicated core/shell/matrix composition profiles.

H. Abe and C. Branton

Membrane Protein Crystallization (MS78)

Although the number of membrane protein structure determinations is growing, each one still requires extensive individual study and membrane protein crystallization continues to be a major bottleneck. This session focused on efforts to improve technology for general applications including the design of new amphiphiles, new concepts for crystallization and experiments with lipid composition. The presentations highlighted recent determinations of physiologically important membrane protein structures, such as the Ca-pump, squid rhodopsin and a human gap junction protein (S. Maeda, Japan). The final presentation, by A. May, USA, concerned a new practical approach, based on microfluidics and showed how diffraction patterns can be obtained *in situ* without any crystal handling. C. Toyoshima (Japan) and T. Kouyama (Japan) described all the steps that allowed them to obtain highly diffracting crystals of Ca-ATPase and squid rhodopsin respectively and the critical role played by lipids selection.

E. Pebay-Peyroula and S. Yoshikawa

New Neutron Sources (MS81)

This microsymposium showcased current developments in neutron sources and their impact on crystallography. It included reports from representatives of each of the three sources that have started produce neutrons in the last two years; the OPAL reactor (Brendan Kennedy, Australia), J-PARC (Yujiro Ikeda, Japan) and the SNS (Ian Anderson, USA). Among the highlights were the world-record power of SNS, the high spatial resolution of the super-HRPD at J-PARC and the high speed of the Wombat diffractometer at OPAL. We also heard about two sources where cold neutron research facilities are being established; the HANARO reactor, (Chang Hee Lee, Korea) and the HFIR reactor (Ian Anderson). Finally, we learned of plans for the development of Europe's next generation neutron source, the ESS-Scandinavia project (Christian Vettier, Sweden). Several important themes emerged during discussion including:

- Are there enough powerful neutron sources to meet the current needs?
- Is there sufficient and timely provision for future neutron sources to satisfy projected future needs?
- How well do current developments in neutron scattering infrastructure meet the changing needs of the community?
- How can outreach activities be improved to attract more users and to promote advances in neutron capability?
- How do we ensure that new sources combine with existing sources to provide competitive service for the community, without dilution of stakeholder support?
- How can research selection programmes be managed to optimise access to the most appropriate user research facilities, particularly when sources are co-located?

These last two points have particular relevance for JAEA in Tokai and for Oak Ridge National Laboratories, where spallation sources are being commissioned at the same campus, and managed by the same organizations, as existing long-serving research reactors.

The session also provided a forum for announcement of the formation of the Asia-Oceania Neutron Scattering Assn, which is intended to co-ordinate of the activities of the neutron scattering societies of the member countries (currently Australia, India, Japan, Korea, Taiwan) and to liaise with the regional neutron scattering societies of Europe and North America on international activities.

Shane Kennedy and Yukio Noda

Space Groups and their Generalizations: A Tribute to E. Ascher and J. J. Burckhardt (MS89)

This microsymposium was organized by the IUCr Commission on Mathematical and Theoretical Crystallography (www.crystallography.fr/mathcryst) to honor two recently deceased Swiss scientists who made important contributions to mathematical crystallography. A. Janner (The Netherlands) reviewed his work with Edgar Ascher (1921-2006) on the derivation of space groups using modern algebraic techniques and on the symmetries of physical systems periodic in space and time, e.g. crystals diffracting an X-ray beam. This research led Janner to describe aperiodic crystals by space groups in higher dimensions, so-called superspace groups. This talk was followed by I. Orlov (Switzerland), who presented an investigation of the 3-dimensional space groups that can be obtained by rational cuts of (3+1)-dimensional superspace groups. P. Zeiner (Germany) investigated subgroups of the space groups and their application to a) phase transitions, b) colour groups, and c) coincidence rotations. B. Souvignier (The Netherlands) reviewed the work of J. J. Burckhardt (1903-2006) on the discovery of the 3-dimensional space group types by Fedorov and Schoenflies and Burckhardt's application of Frobenius congruencies to obtain general results on space groups in N dimensions and to derive the types for 2 and 3 dimensions in a systematic way. Y. Teshima (Japan) investigated the packing densities and space groups of self-supporting 3-fold periodic packing of congruent circular cylinders, which he nicely illustrated with wooden models.

Hans Grimmer and Massimo Nespolo

AWARDS AND PRIZES

IUCr XXI Congress Poster Prize Winners



RCSB PDB



Chaille T. Webb

Chaille T. Webb (Australia), 'Structural insights into the mitochondrial import complex, TIM9.10'.



CCDC



CCDC winner

Ana E. Platero-Prats (Spain), 'Design of new MOFs based on alkaline earth metals with promising catalytic applications'; Laura J. McCormick (Australia), 'The diabolcules: Some unexpected copper clusters'; and Christophe M. L. Vande Velde (Belgium), 'Charge density of $\text{Ni}(\text{MePh}_2)_2(\text{C}_6\text{F}_5)_2$ (1) and the energy density in the Ni-C bond'.



Oxford Cryosystems Low Temperature

Helena J. Shepherd (UK), 'Structural studies of spin crossover compounds under extreme environmental conditions'.

Zeitschrift für Kristallographie

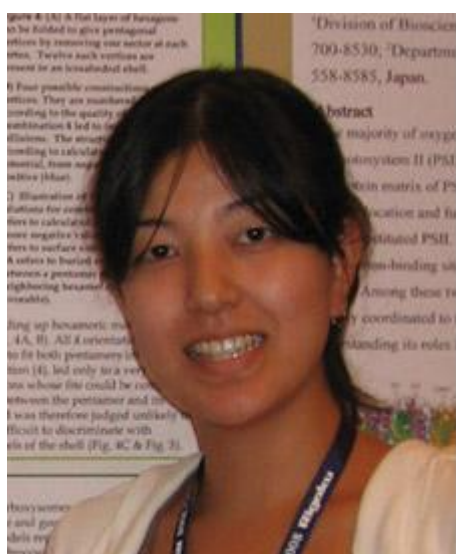
Marek Pasciak (Poland), 'Multi-resolution atomistic simulations and diffuse scattering in BaTiO_3 '.

EMU

Mihoko Hoshino (Japan), 'First report of natural oxyallanite: Oxidation and dehydration during welding of volcanic tuff'.



IUCr



(L) Shiho Tanaka (R) Kevin H. Stone

Kevin H. Stone (USA), 'Structure solution of $\text{Ag}(\text{pyz})_2\text{S}_2\text{O}_8$ in the presence of impurity phases using robust refinement'; Shiho Tanaka (USA), 'Atomic-level models of the bacterial carboxysome shell'; and Tatsuhiro Kojima (Japan), 'Solvent driven association and dissociation of the hydrogen-bonded protonated decavanadate dimer'.



CrSJ



CrSJ winners

Yoshihisa Ishikawa (Japan), 'Single crystal structure analysis by neutron 2D-PSD'; Felipe Gandara (Spain), 'A rare-earth MOF series: Fascinating structure, efficient light emitters and promising catalysts'; Alexandra K. Wolf (Germany), 'Prediction and experimental determination of the crystal structure of SiBr_4 '; Amit Delori (India), 'pKa directed host-guest assemblies of 2,4-diamino-6-methyl-triazine with various dicarboxylic acids'; Norifumi Muraki (Japan), 'Structure of protochlorophyllide reductase reveals a mechanism for greening in the dark'; Yi-Wei Chang (Taiwan), 'Crystal structures of the 70-kDa heat shock proteins in domain disjoining conformation'; Not Shown: Tatsuki Tadenuma (Japan), 'Study of spin and orbital magnetic form factors of CeRh_3B_2 by X-ray magnetic diffraction'; Shigeyuki Morishita (Japan), 'Image reconstruction by a combination of diffractive imaging and selected area nano diffraction'; and Tatsuya Ibuki (Japan), 'X-ray analysis of FliJ, a cytoplasmic component of the flagellar type III protein export apparatus'.

CrystEngComm



CrystEngComm winner

Sayon A Kumalah (USA), 'Properties of metal-organometallic frameworks derived from facially η^6 metalated terephthalates'; Sudarshan Mahapatra (India), 'A novel approach to specifically crystallize anhydrous compounds: Crystal structure of adenine'; Yute Kin (Japan), 'Chiral recognition for inclusion compounds of 3-epicholic and 3-epideoxycholic acids with alcohols'; Gregory J Halder (USA), 'In situ X-ray diffraction studies of host-guest properties in nanoporous spin crossover frameworks'; and Ching-Yi Wei (Taiwan), 'Structure and magnetic properties of a iron(III) spin crossover complex'.

MEETING REPORT

French Crystallographic Association Meeting



Rennes, France, July 2008



Clockwise from top left: Welcome speech by Jean-Claude Daran; the town hall reception; the conference dinner.

The meeting was held at the U. of Rennes, a 2000-year old city with a rich architectural heritage and charming mediaeval streets. The conference was organized in three plenary sessions and two parallel sessions of five mini symposia. Topics included Modeling of Aperiodic Crystal Structures, the Formation of Limestone by Invertebrates, Technological Revolutions (Methods, sources and detection), Time-resolved Structures and Structures and disorders. The mini symposia covered Imagery and Nanometric Diffraction, Signalisation and Cellular Regulation, Crystallochemistry, Infections, Compounds of Pharmacology Interest, Proteins and Membranes, Coupled Characterization, Compounds of Biomedical Interest, Surface and interface and Structural Biology under Extreme Conditions. A session on the

teaching of crystallography was also organized.

The 101 posters were displayed for the whole meeting in a large area close to the coffee. In total, 270 delegates from France, Algeria, Morocco and Tunisia attended the conference and 4 students and young scientists received sponsorships from the AFC (French Assn of Crystallography). The local committee organized a warm welcome reception in the town hall and a conference dinner was held in one of the most famous restaurants of Rennes. Financial support provided by exhibitors was greatly appreciated. The next meeting will be held either in Strasbourg or Lyon in the summer of 2010.

Jean-Claude Daran, AFC President

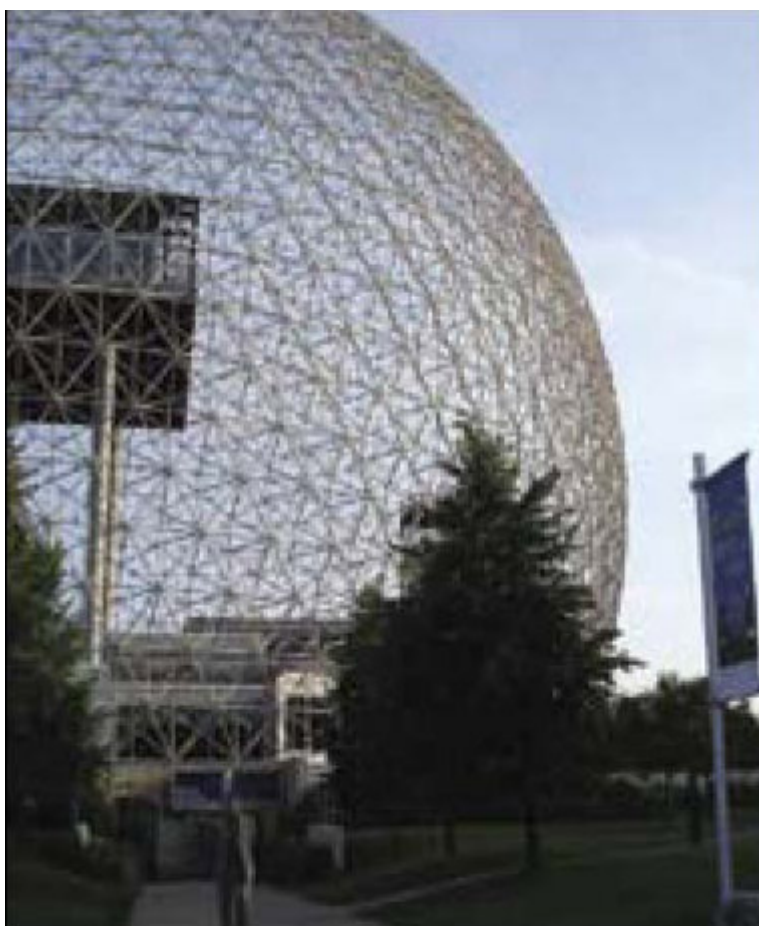
MEETING REPORT

37th Assembly of COSPAR



Montreal, Canada, July 2008

<http://cosparhq.cnes.fr/>



Biosphere Museum, Montreal, Quebec



Gerda Horneck, Chair of the COSPAR Landesausschuss of the DFG and Hanna Dabkowska, IUCr representative to COSPAR.

The Committee on Space Research (COSPAR) was established in 1958 by the International Council of Scientific Unions (now the International Council for Science) with its main objective to promote international collaboration on various levels in scientific research in space, with an emphasis on the exchange of results, information and opinions. Developing world standards for the protecting space requires the cooperation of national and international organizations and specialists working in this area.

The majority of COSPAR activities are devoted to space topics (astronomy, space travel and exploration or climate research). The most interesting for the IUCr division of COSPAR, the Scientific Commission on Materials Science in Space (MSS), deals with scientific experiments in materials and fluid sciences that utilize the physical conditions of space (mainly reduced gravity). Experiments on the growth of crystals in microgravity were, at some point, also part of these programs. The MSS Commission reviews fundamental theoretical and experimental approaches, helping to understand emerging fields, and it recommends promising avenues for future research. It also coordinates exchange of information on scientific subjects. This Commission is chaired by V. Shevtsova (Belgium), with vice-chairs W-R. Hu (China), S. Amiroudine (France) and S. Yoda (Japan).

'Advances in Space Research' (ASR - <http://ees.elsevier.com/as>), an official journal of COSPAR, covers all areas of space research including, but not limited to, space studies of earth surface, meteorology, climate, fundamental physics in space, materials physics in space, space debris, weather and earth observation of space phenomena. ASR is included in the Web of Science and related indexes and, thanks in part to a huge increase in downloads (from 35,000 in 2002 to 279,000 in 2007), now has an impact factor of 0.774, the highest in its history and it expected to continue to rise. All COSPAR Associates to consider ASR as the journal for their future papers.

The COSPAR President is R.-M. Bonnet (France) and the Vice-Presidents are W. Hermesen (Netherlands) and E. C. Stone (USA). Members of the Bureau are: M.-H. Jiang (China), M. E. Machado (Argentina), G. G. Shepherd (Canada), R. Sridharan (India), L. Zelenyi (Russia) and J. B. Zielinski (Poland).

The local Organizing Committee, headed by G. G. Shepard (Canada) did an excellent job. A total of 2464 participants were in attendance including almost 350 students. 3775 abstracts were submitted (by 2874 authors) and 3754 were accepted. The final program consisted of almost 2500 oral presentations and over 1000 posters. The 50th Anniversary Lectures were presented by Peter Willmore (UK - '[COSPAR's First 50 Years](#),'), by Stefano Vitale (U. of Trento and INFN - '[Space and the Spacecraft as a Precision Laboratory](#)') and by L. A. Fisk (USA - '[The Impact of Space on Society](#)'). All the participants from around the world had very good time in beautiful Montreal. The full scientific program of the Montreal Assembly may be viewed at <http://cosparhq.cnes.fr/>.

The next COSPAR Assembly will be held in Bremen, Germany in 2010.

Hanna Dabkowska, IUCr representative to COSPAR

MEETING REPORT

Remembering Cruickshank

Manchester, UK, November 2007



Speakers at the D W J Cruickshank Memorial Symposium held in the Whitworth Hall of the University of Manchester; left to right: Keith Moffat, Chick Wilson, Garib Murshadov, Mike Dacombe, Giuseppe Fillipini, Bob Gould, Helen Stuckey (daughter), Alajos Kalman, John Cruickshank (son), Bob Munn, Louise Johnson and John Helliwell.

John Helliwell and Bob Munn (Manchester U.) organized a mini-symposium to celebrate life and achievements of Durward W. J. Cruickshank (1924-2007) in Manchester, November 2007. Among the 100 or so participants was Farid Ahmed (Ottawa), DWJC's first research student at Leeds U. and co-author of papers in 1952 and 2007. Farid commented touchingly on Cruickshank's faith, recognized by a hymn and prayer opening the meeting.

While Cruickshank is most widely appreciated in the area of determination, refinement and precision of molecular structures, the breadth of his scientific achievements embraced quantum chemistry, inorganic

oxyanion bonding, gas-phase electron diffraction, anisotropic thermal vibrations, aromaticity, Laue diffraction and proteins, not to mention history and biography. The remarkably high average of citations per publication was noted. Alajos Kalman (Budapest U.) expanded the theme of tetrahedral oxyanions, while another onetime post-doctoral collaborator from 1970, Giuseppe Filippini (ISTM-CNR and Milan U.), made some philosophical observations and was a reminder of Cruickshank's continuing interest in hydrocarbons, reflected more fully in the publications in the *J. Mol. Structure* special issue (**130**, 1-191, 1985).

Keith Moffat (Chicago U.) spoke of his collaboration with himself and Helliwell at Daresbury and York U. (1985) with a 1909 (pre-X-ray-diffraction) reference to crystallography of haemoproteins. Laue photography, largely discarded after painstaking use by Pauling and Wyckoff in the 1920s, was revived by the availability of intense polychromatic radiation in the 1980s. Intensive work and spirited discussion among the trio led to the solution of the problem of overlapping orders and to the exploitation of short exposure times in the study of proteins and viruses. Louise Johnson (Biophysics, Oxford U.) described Cruickshank's contribution to enzymology through difference maps and time-resolved studies based on the Laue technique. Garib Murshadov (York U. and CCP 4) spoke about REFMAC for protein refinement, the Cruickshank dispersion precision indicator and the contemporary impact of early Cruickshank papers.

Glasgow's recognition of Cruickshank was illustrated by Chick Wilson (Glasgow U.), while Bob Gould (BCA) and Mike Dacombe (IUCr) recalled his contributions respectively to the British Crystallographic Assn and to the IUCr.

The most moving presentation was the voice of Cruickshank recorded, only days before his death, in an interview by Martyn Clark (Leeds Computer Society). Apparently Kathleen Lonsdale's public lectures on reciprocal space proved tough for a young engineering graduate working at Naval Intelligence in London. However, having to do engineering at Loughborough during WWII, instead of mathematics at Cambridge, proved a blessing. Cruickshank's appointment in 1946 as assistant to Gordon Cox at Leeds U. was initially to utilise redundant military X-ray equipment to improvise devices to aid structure-factor calculation and Fourier synthesis. Thanks to George Jeffrey, DWJC saw papers on the wartime research of Andrew Booth (who had worked for Cox and later went to Canada). These (summarised in *Fourier Technique in X-ray Organic Structure Analysis*, Cambridge U. P., 1948) described novel approaches to refinement by sections and differential syntheses, finite-series corrections, and accuracy estimates, developments of which led to an *Acta* note in 1948, a paper in 1949 and the DWJC series in the 1950s. Use of Beevers-Lipson strips and punched cards at Leeds gave place to five years of weekly overnight runs with Ahmed and Diana Pilling on the Manchester U. electronic computer and ultimately to the successful bid for installation of the Ferranti Pegasus computer at Leeds in 1958.

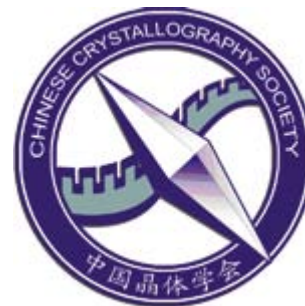
Many of Cruickshank's family attended the meeting, which was formally opened and closed by his son John Cruickshank. Though there was no contribution on golf, Durward's other serious non-science pursuits of genealogy and extreme travelling were outlined by his daughter Helen Stuckey. DWJC's parents were medical doctors who met in London. His extensive searches (including visits to Salt Lake City, USA) on the maternal side showed that the family came from villages in the district close to Manchester where DWJC spent his later life. They also revealed ancestral links with the poet William Wordsworth (b 1770) and a Yorkshire mathematician and school benefactor, John Hymers (b 1803). Cruickshank made several cruises to the Arctic (close to the course near Baffin Island of a Yorkshire whaling skipper forebear) and the Antarctic (crystallographic names encountered in Crystal Sound are given in *IUCr Newsletter* **8** [3] 25, 2000).

The symposium formed a fine farewell to a courteous, friendly and genuine scientist who for 60 years worked to make substantial advances across a wide range of crystallographic science.

Derry W Jones

MEETING REPORT

CCrS 4th General Assembly



CCrS 4th General Assembly

Huangshan City, Anhui, China, July 2008



Photograph of the first board meeting of the 4th CCrS congress

The 4th General Assembly of Chinese Crystallographic Society (CCrS) took place July 27-30, 2008 in Huangshan city, China, near the scenic Huang Shan mountain ridge. The General Assembly was accompanied by the academic conference, in which plenary lectures were delivered by Yigong Shi, Ze Zhang, Jiyang Wang, Xiaoming Chen, Zhenhong Mai, and Thomas Blanton (ICDD, USA). Over 120 oral talks were given in 4 conference halls on the topics of: Biological macromolecular structures; Small molecular structures; Powder diffraction methods; and Crystal growth and characterization, fields of the four academic commissions of the CCrS. Over 500 participants (half students) from throughout China attended the meeting, including some industry exhibitors. The general board committee members of CCrS were re-elected by the majority vote of the participants, and the board committee members held a meeting to elect the standing committee members and the president of CCrS. The first board committee meeting was attended by Jiutong Chen, Xiaolong Chen, Xiaoming Chen, Jianping Ding, Yuhui Dong, Yunlong Feng, Jianhua He, Hong Ji, Yizhi Li, Libing Liao, Jian-Hua Lin, Shixiong Liu, Zhijie Liu, Yang Lv, Zhenhong Mai, Liwen Niu, Feng Pan, Lianmao Peng, Yuanyuan Qiao, PC Shaw, Yuequan Shen, Haibin Song, Chengyong Su, Xiao-Dong Su, Maikun Teng, Cong Wang, Dacheng Wang, Jiyang Wang, Yingxia Wang, Zhanshan Wang, Zheming Wang, Linhong Wong, Xiaoshan Wu, Xintao Wu, Yicheng Wu, Dongfeng Xue, Deren Yang, Ning Ye, Changcheng Yin, Lingmin Zeng, Ze Zhang, Yanming Zhao, Hegeng Zheng, Weitao Zheng, Shifu Zhu. And the Secretaries, Na Yang and Chong Chen have also participated in the meeting. The first board committee meeting elected the following standing committee members (22 in total). The standing committee is the decision body of CCrS daily operation and the members are (names are arranged alphabetically): Xiaolong Chen (Inst. Of Physics, CAS), Xiaoming Chen (Zhongshan U), Jianping Ding (SIBS, CAS), Weiming Gong (IBP, CAS), Luhua Lai (Peking U.), Jian-Hua Lin (Peking U.), Shixiong Liu (Fuzhou U.), Yang Lv (Chinese Acad. of Medical Sciences), Zhenhong Mai (Inst. Of Physics,

CAS), Liwen Niu (USTC), Feng Pan (Tsinghua U.), Lianmao Peng (Peking U), Zihao Rao (Nankai U), Yigong Shi (Tsinghua U.), Xiao-Dong Su (Peking U.), Mu Wang (Nanking U.), Dacheng Wang (IBP, CAS), Jiyang Wang (Shandong U.), Zheming Wang (Peking U.), Yicheng Wu (CAS), Ze Zhang (Beijing U of Technology), Weitao Zheng (Jilin U).

Chairs and Vice-Chairs of the six commissions of the 4th CCRS congress

Commissions	The 4 th CCRS	
	Chair	Vice-Chairs
Small Molecular Structure	Xiaoming Chen	Zheming Wang
Macro-molecular Structure	Dacheng Wang	Liwen Niu
Powder Diffraction	Xiaolong Chen	Lingmin Zeng, Libing Liao
Crystal Growth & Characterization	Yicheng Wu	Mu Wang
Electron Diffraction	Lianmao Peng	Ze Zhang
Crystallography Education & Popular Science	Shixiong Liu	Xiao-Dong Su, Yang Lv.

At the board committee meeting, Jian-Hua Lin (Peking U.) was elected president of the 4th CCRS congress, Xiao-Dong Su (Peking U.) was elected Vice-President and the Chairpersons of six commissions were also elected (see above).

Xiao-Dong Su, Secretary-general, Chinese Crystallographic Society

AWARDS AND PRIZES

2009 Aminoff Prize



George Sheldrick



Gérard Bricogne

The Royal Swedish Academy of Sciences (RSAS) has decided to award the 2009 Gregori Aminoff Prize in crystallography to George M. Sheldrick (Göttingen, Germany) and Gérard Bricogne (Cambridge, UK) 'for their contributions to theoretical development and methodological implementation in crystallography'. Crystallographic methods are used to determine the positions of the atoms in semiconductors as well as in virus particles. The 2009 laureates have both contributed to make the methods of crystallography more powerful and more generally applicable.

George Sheldrick (Georg-August Universität, Göttingen, Germany) has developed the software package SHELX, which early began to dominate structural determinations of smaller molecules. Through continuous development and enhancement SHELX has today become a powerful and easy-to-use tool within all scientific disciplines that uses structural information -- from mineralogy to molecular medicine. Because SHELX is free to use it has had a tremendous impact among researchers worldwide.

Gérard Bricogne (Global Phasing Ltd, UK) has contributed to the development of crystallographic methods and thus revolutionized the research area for determination of the structure of biological macro molecules. In 1978 he succeeded for the first time to determine virus structures at an atomic scale. He founded the non-profit company Global Phasing Ltd, which today, free-of-charge, provides researchers with software for crystallographic methods.

The Prize will be awarded by the Royal Swedish Academy of Sciences on March 31, 2009. The prize amount (SEK 100 000) is to be equally divided by the two laureates.

NOTICE

StrucClues Site Team

In 2004-2005, more than a few members of the international crystallographic community were kind enough to contribute their comments on certain empirical 'cases' presented at a short-lived web site called StrucClues.

The StrucClues Site Team is now pleased to report that this website has recently been revived at: <http://strucclue.ornl.gov> and new 'cases' will begin accumulating shortly.

Following the same protocol used back in 2004-2005, publication of each new 'case' at StrucClues will be followed by an email to one or more of the people involved in the original depositions of the PDB structures that constitute the new 'case'. This email will solicit comments of the same type that can currently be seen for many of the existing cases at StrucClues.

And therefore, the StrucClues Site Team is hopeful that members of the crystallographic community (and their non-crystallographic colleagues) will continue to respond to StrucClues emails with the same remarkable generosity of spirit that they have previously exhibited.

David Halitsky

AWARDS AND PRIZES

2008 McMurdie Award



Jeffrey Dann (left) with ICDD Chairman Thomas Blanton

The International Centre for Diffraction Data is pleased to announce that long-time ICDD member, Jeffrey Dann of Global Tungsten & Powders (formerly OSRAM Sylvania), Tonawanda, PA, was named as the 2008 McMurdie Award Recipient. The award itself was presented at the 57th Annual Denver X-ray Conference, held in Denver, Colorado. The award recognizes distinguished work which improves the Powder Diffraction FileTM (PDF).

Since 1976, Jeff has been an active participant of the Metals & Alloys Subcommittee and Task Team and has served as Chairman of the Target Systems Subcommittee responsible for identifying materials missing from the PDF and making recommendations to the Grant-in-Aid Committee to promote proposals focusing on these missing phases.

NOTICE

Crystallographer of Note

John Kuriyan, Chancellor's Professor of Molecular and Cell Biology and Chemistry, University of California, Berkeley; Investigator, Howard Hughes Medical Institute was elected to membership in American Academy of Arts and Sciences.

MISCELLANY

Life in Crystals

An Italian research team found ancient pollen sealed in the colossal crystals in a lead and silver mine in northern Mexico. The team, led by mineralogist Paolo Forti (U of Bologna, Italy), suspected that the selenite crystals, some as long as 11 meters, could contain pollen that was in the area when they formed several hundred thousand years ago.

The pollen may help scientists reconstruct ancient climates and vegetation cover in the northern region of the Chihuahua desert. Forti's team is now using radiometric dating to get a definitive age for the crystals.

From Random Samples, Constance Holden, ed.

AWARDS AND PRIZES

Additional ECM24 Poster Prizes

A list of the ECM24 poster prizes was reported in Volume 16, Number 1.

The following awards were also presented at the meeting:

- RSCB Protein Data Bank: Humberto Couto Fernandes (Poland), 'Yellow lupine pathogenesis-related protein as a reservoir for cytokinins'.
- *Zeitschrift Für Kristallographie*: Oliver Oeckler (Germany), 'Crystal chemistry of disordered layer-like oxonitridosilicates'.
- EMU: L. A.Pajdzik (UK), 'Three-dimensional birefringence imaging of optically anisotropic materials'.

MISCELLANY

Crystallography and the Nobel Prize

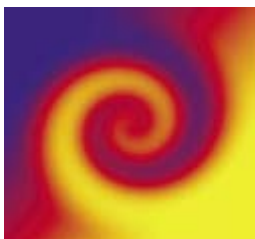


There have been 12 Nobel Prizes in chemistry and physiology or medicine awarded for work in the field of crystallography from 1956 to 2006. Almost one in four chemistry prizes since 1956 have been for structure work, and in the last decade fully half have dealt with work related to macromolecular structure. From 1970 to 2006, 4% of all chemistry publications dealt with crystallography, yet this subfield captured 19% of the available Nobel Prizes. During the past decade, crystallography papers represented 7% of all chemistry publications, but commanded 4 of 10 available prizes. Overall, the Nobel Prizes in chemistry are noticeably enriched for work in macromolecular structure determination. Macromolecular structure determination is a potent tool to understand biological systems and periodically yields landmark results that impact the scientific community at large. It would also seem that the surest road to Stockholm is through a crystal tray.

From a letter from Michael Seringhaus and Mark Gerstein, Science, January 2007 (Vol. 315, p. 412).

REGIONAL NEWS

Cuban Hurricane Damage



Cuba was seriously damaged by two huge hurricanes in September 2008. Whole regions of the country were devastated and hundred of thousands of houses have been damaged or totally destroyed. In the middle of the destruction educational facilities struggle to serve their students. We have to make our universities stronger and better and to graduate more skillful professionals that can better serve their country.

In our institute we are assessing damages and discussing what to do. Our buildings did not suffer too much but some of our scientific equipment, already poor and outdated, will not survive this blow as they have been soaked in water and in our tropical climate corrosion will unavoidably render them useless. Parts of the ceiling were blown away in one of our buildings and air conditioner and acclimatization equipment was partially damaged.

We would like through the IUCr, to ask our colleagues in crystallography around the world to help us as much as they can. Any help in infrastructure, equipment or financial resources is welcomed. The goal is to rebuild our crystallography laboratory that is the only one in Cuba Universities. We strongly believe that even in crises a country must build for the future.

We will go on as planned with our crystallography school for July 2009. Every two years we organize an international school on crystallography where students from Cuba and Latin America hear state of the art lectures presented by invited experts in the field. This school has been an important part in the curricula in physics, material science, chemistry, engineering and life science. We ask professors who are willing to come to our school covering their cost and give lectures to please contact me so we can arrange the school program. We would like this year to emphasize protein crystallography, from single crystal to recent developments in powder methods.

I take the opportunity to thank you personally for the friendly support over the years.

Ernesto Estevez Rams, U. de la Habana

NOTICE

International Cooperation



On September 25, 2007 in Ottawa, an agreement was signed by the Government of India with the Canadian Light Source (CLS) and the Univ. of Saskatchewan to promote cooperation between India and Canadian researchers in synchrotron science. The agreement opens the way to explore joint projects including materials research, earth and environmental sciences, and biomedical and life sciences. Other opportunities may see Indian researchers traveling to the CLS as customers to use the facility, as well as to learn about their operation and design of experimental equipment. For the full press release please go to www.lightsource.ca/media/media_release_20070925.php.

A Canadian/German team is developing soft X-ray spectroscopy as a new tool for the investigation of one of the key areas of soil science: the chemistry of nitrogen. Collaborators from the Universities of Saskatchewan (Fran Walley) and Rostock (Peter Leinweber) have combined to produce the necessary first step, a reference fingerprint library to determine the nature of unknown nitrogen in environmental materials (see Leinweber *et al.* 2007, journals.iucr.org/s/issues/2007/06/00/issconts.html). This is part of the commitment of the CLS to accommodate 'dirty' real-world samples that has also brought researchers from the USA and Australia to Saskatoon.

REGIONAL NEWS

AACr News

The 4th meeting of the Asociación Argentina de Cristalografía (AACr) was held in Bahía Blanca south of Buenos Aires. The program included powder diffraction (chemists and mineralogists) and Protein Crystallography (Physics). The 45 participants included people working at the synchrotron facility in Brazil and the Pasteur Institute at Montevideo, Uruguay, and 16 graduate students from Argentina. We have a new president, vice president and secretary. The new treasurer elect will share responsibilities with the old one for the next year.

Future meetings are planned for Posadas, near the Iguazú Falls (2009), in Buenos Aires (2010, the bicentenary of Argentina), Bariloche (2011) and in Montevideo, Uruguay (2012).

La Plata will soon host several new instruments related to crystallography including new single crystal diffractometers. A group of geologists has been awarded a powder diffractometer, a group of physics and chemists was awarded an instrument to do EXAFS and XANES and a group of engineers an electron microscope. Two Diffractometers for Protein work have been received as donations, one in Buenos Aires and one in Rosario. It seems that Crystallography may soon flourish in Argentina.

AWARDS AND PRIZES

CrSJ General Assembly



(left to right) M. Fujihashi, M. Yashima, A. Takenaka (President), and J. Kondo.

IUCr2008 was held in Osaka, Japan, so the 2008 General Assembly of the Crystallographic Society of Japan was held at Grand Cube Osaka on August 27 during the Congress. At the Awards Ceremony, the Prize for Science in Crystallography went to M. Yashima (Tokyo Inst. of Technology). The Young Crystallographer Awards went to M. Fujihashi (Kyoto U.) and J. Kondo (U. Louis Pasteur). At the general meeting, N. Yasuoka (Prof. Emer. Himeji Inst. of Technology), F. Iwasaki (Prof. Emer. The U. of Electro-Communications), and M. Tanaka (Prof. Emer. Tohoku U.) became Honorary Members of our society.

Tsuyoshi Inoue

LETTER TO THE EDITOR

Letter to the Editor

To the Editor:

The book review by Derry W. Jones (*IUCr Newsletter*, (2008) V16, n2, 21), ends with, 'Crystallographers who have not read any of Watson's recent books should sample this one first.' This crystallographer and a retired chemistry professor is shocked that the latest book by 'HONEST JIM' is accorded the honor to be reviewed in the International newsletter devoted to Crystallography in all its manifestations.

James D. Watson is not, never was a crystallographer in any sense of the discipline, not even on the fringes far removed from any possible remote relationship to crystallography. Worse yet, he was abysmally ignorant of any aspects of chemistry involving purines and pyrimidines as is evident from the sketches, drawn by him in his book 'The Double Helix', of guanine, adenine, thymine and cytosine. One must give credit to 'Honest Jim' for explicitly though belatedly acknowledging, in one of his seminars away from Cold Spring Harbor, that there was another person deserving of a Nobel Prize for the elucidation of the three dimensional structure of DNA, at the molecular level. It was none other than Jerry Donohue.

Even after adding the Epilogue to his original 'The Double Helix', he never gives full credit to the far superior crystallographic knowledge Rosalind Franklin had and he was fully aware of the helical nature of the structural features based upon her experimental X-ray diffraction work on the sodium salt of DNA fibres.

Brahama D. Sharma