

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

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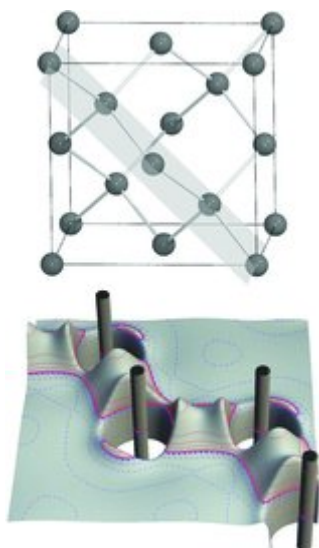
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Multipole electron-density modelling of synchrotron powder diffraction data: the case of diamond

Acta Cryst. (2010). A66, 458-469 (doi.org/10.1107/S0108767310014236)



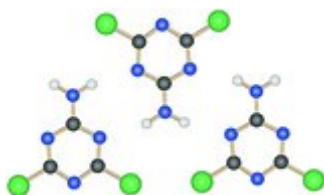
Accurate structure factors have been extracted from synchrotron powder diffraction data measured on crystalline diamond. A multipole-model division of overlapping reflection intensities is introduced to limit the spherical-atom bias of conventional Rietveld refinement models. The structure factors are subsequently used for multipole electron-density modelling and a detailed comparison is made with results from *ab initio* theory. The high quality of the data facilitates a demonstration of the correlation between electron density and thermal parameters even for light atoms.

H. Svendsen, J. Overgaard, R. Busselez, B. Arnaud, P. Rabiller, A. Kurita, E. Nishibori, M. Sakata, M. Takata and B. B. Iversen

IUCR JOURNALS NEWS

The lines-of-force landscape of interactions between molecules in crystals; cohesive versus tolerant and 'collateral damage' contact

Acta Cryst. (2010). B66, 396-406 (doi.org/10.1107/S0108768110008074)



A motif in the crystal structure of QIZHIQ [Archer, Goldberg, Lynch & Krische (2000). *J. Am. Chem. Soc.* **122**, 5006]: N—H...N (blue-white-blue) hydrogen bonding brings collateral Cl...Cl (green-green) contact down to 3.29 Å. The interaction energy over this short contact is but slightly repulsive. Drawing by SCHAKAL (E. Keller).

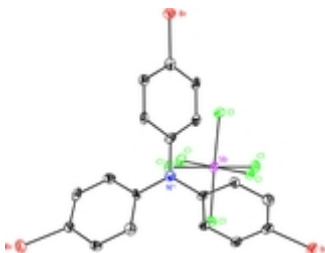
Calculation of interaction energies between pairs of molecules in organic crystals shows as expected that intermolecular contact does not always occur at minimum energy, but also, somewhat unexpectedly, that short approach is very often irrelevant in terms of energy, and sometimes even repulsive. Caution should be exerted when analyzing crystal structures in terms of 'the shorter, the stronger' bonding criteria for atom-atom contacts.

A. Gavezzotti

IUCR JOURNALS NEWS

Tris(4-bromophenyl)aminium hexachloridoantimonate ('Magic Blue'): a strong oxidant with low inner-sphere reorganization

Acta Cryst. (2010). C66, m171-m173 (doi.org/10.1107/S0108270110019748)

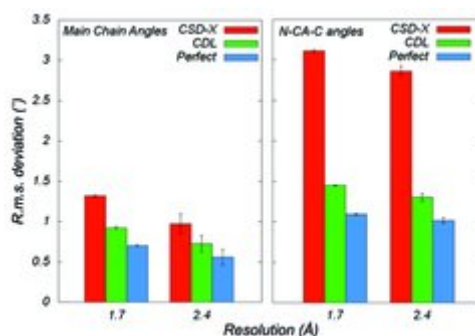


The commercially available amine radical cation tris(4-bromophenyl)aminium hexachloridoantimonate, dubbed 'Magic Blue', is prized by chemists for its high oxidation potential and its propensity to undergo simple electron transfer reactions. Structural studies of the neutral triarylamine and its radical cation show that the bond distances and angles are almost identical in the two species. This small degree of structural rearrangement on electron transfer contributes to the kinetic efficiency of Magic Blue as an oxidant.

M. Quiroz-Guzman and S. N. Brown

Using a conformation-dependent stereochemical library improves crystallographic refinement of proteins

***Acta Cryst.* (2010). D66, 834-842 (doi.org/10.1107/S0907444910019207)**



Plots of the main chain (left panel) and N—Ca—C (right panel) r.m.s. bond angle deviation from ideality as a function of the restraint library in test refinements at 1.7 Å and 2.4 Å resolution. CSD-X is the Engh & Huber library and CDL is the new conformation-dependent library. The improved geometry agreement was obtained with no significant change in *R* factors.

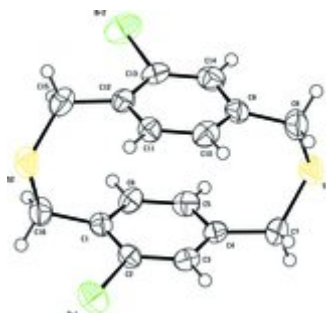
A conceptually novel restraint library with ideal geometry targets parameterized by ϕ, ψ strongly outperformed the commonly used Engh & Huber library and approached the performance of a 'perfect' library derived from a 1.05 Å resolution model of the test case protein. The results imply that more accurate protein structures at all resolutions will be obtained when refinement packages are modified to account for this new paradigm of ideal geometry functions.

D. E. Tronrud, D. S. Berkholz and P. A. Karplus

IUCR JOURNALS NEWS

6,14-Dibromo-2,11-dithia[3.3]paracyclophane

***Acta Cryst.* (2010). E66, o2123 (doi.org/10.1107/S1600536810028874)**

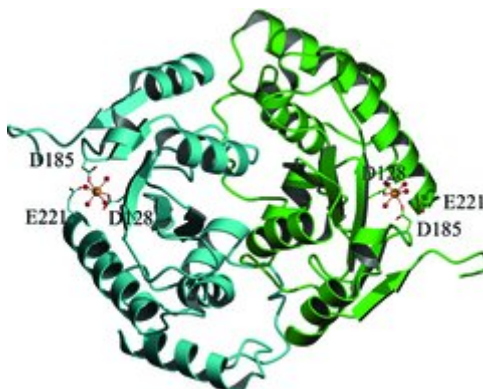


The crystal structure of $C_{16}H_{14}Br_2S_2$ was determined as a contribution to a structural study of dithia[3.3]paracyclophane derivatives with bromine substituents. The short distance of 3.313 (5) Å between the centroids of the two benzene rings is less than the normal packing distance (3.4 Å) between aromatic rings in organic compounds, thus supporting potential transannular π - π interaction between the rings in the cyclophane unit. The crystal packing exhibits weak intermolecular S...S contacts of 3.538 (2) Å.

X. Zhu and M. Hu

Structural studies of the catalytic core of the primate foamy virus (PFV-1) integrase

***Acta Cryst.* (2010). F66, 881-886 (doi.org/10.1107/S1744309110022852)**



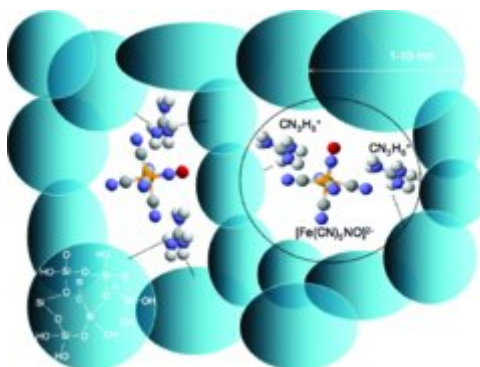
Structure of the dimer of PFV-1 integrase catalytic core with manganese (orange sphere). The residues of the catalytic triad are shown as ball-and-sticks. Water molecules involved in manganese ion coordination are shown in red.

Integrases are key enzymes for the integration of retroviral genomes into host cell DNA. Cations, either Mg^{2+} or Mn^{2+} , bound to the catalytic core which carries the catalytic triad D-D35E, are essential for all activities of the protein. We determined structures of the catalytic core of the human foamy virus with and without Mg^{2+} and Mn^{2+} , which show the effect of cations on the conformation of the active site and thus give hints into the catalytic mechanism.

S. Réty, L. Rezábková, B. Dubanchet, J. Silhán, P. Legrand and A. Lewit-Bentley

Identification of single photoswitchable molecules in nanopores of silica xerogels using powder diffraction

J. Appl. Cryst. (2010). 43, 1040-1045 (doi.org/10.1107/S0021889810028955)

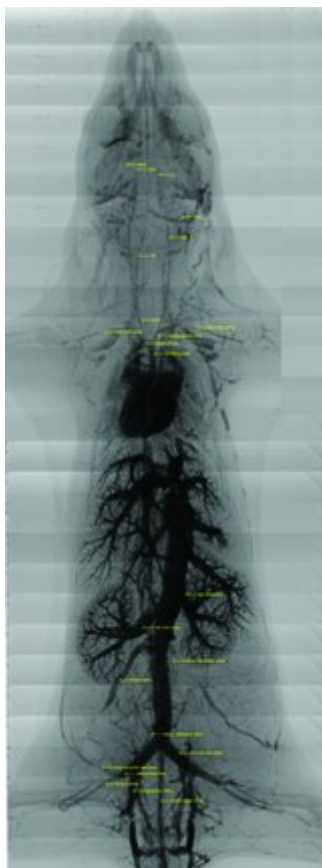


Nanostructured functional materials are often realized by embedding functional molecules in porous host materials. We demonstrate that powder diffraction experiments combined with the Debye approach enable us to extract structural information of isolated molecules in a host: the structural motif (fingerprint) of the molecule, the pore filling factor and the main distances between host and guest material. This opens the way to structural characterization of such amorphous composite or hybrid materials with standard laboratory diffractometers.

A. Cervellino, J. Schefer, L. Keller, T. Woike and D. Schaniel

Microvascular imaging using synchrotron radiation

J. Synchrotron Rad. (2010). 17, 517-521 (doi.org/10.1107/S0909049510018832)



Synchrotron radiation X-ray angiography of a mouse showing the mouse blood vessels in the whole body. In vascular diseases, visualization of microvasculatures is an important step in understanding the mechanism of early vessel disorders and developing effective therapeutic strategies. However, the microvessels involved are beyond the detection limit of conventional angiography. A new angiography system, synchrotron radiation microangiography, has been developed. Iodine and barium sulfate were used as blood vessel contrast agents. Dynamic angiography in mouse brain was performed with a high spatial image resolution of 20-30 μm . Physiological features of whole-body mouse microvasculature were investigated for the first time.

P. Liu, J. Sun, J. Zhao, X. Liu, X. Gu, J. Li, T. Xiao and L. X. Xu

SPECIAL REPORT

Crystallography in Spain

Some historical and general outlines



A sample of Lapis specularis.

Spain has been linked to crystals for centuries as the home of important mining ore deposits. The first Spanish contribution to the history of crystals was reported by Pliny the Elder (I Century AD) in his 'Natural History', where he describes the windows and greenhouses of the richer inhabitants of the Roman Empire being covered by crystals of 'Lapis specularis', the Latin name for large transparent crystals of gypsum. This dehydrated form of calcium sulphate was extracted by Romans in Segóbriga (La Mancha) because of its crystal clarity, size (up to one meter) and perfect flatness.



Deposits of Lapis specularis in Segóbriga.



Top: A view of La Alhambra, Granada (XIII Century). Bottom: Sample of mosaics in La Alhambra, Granada (XIII Century).

The vast amount of mineralogical information contained in Pliny's 'Natural History' was preserved and enhanced in 'Book XVI on Stones and Metals' which covered the Etymologiarum of Isidor of Seville (560-636). It is also in the Lapidarium of Alfonso X (1221-1284), a fascinating work by a group of Muslim, Hebrew and Christian sages from a time when peaceful multicultural collaboration was demonstrated to be possible. Nevertheless, it was the unparalleled talent of the Arabian geometers in investigating the problem of tessellation of two-dimensional space, which made the most important pre-Renaissance Spanish contribution to crystallography and geometrical art. The decorative symmetry of the tiling in the Alhambra Palace in Granada is today used to teach symmetry all over the world.

Several hundred years later, in the 15th century, we find many examples of interest in bi-dimensional structures and symmetry, as is found on the ceilings of the main rooms of castles, palaces and special buildings such as the U. of Alcala or Segovia's Castle, near Madrid.

The variety of products found in Spanish mines and the enormous richness of American ores motivated the work of excellent metallurgists and mineralogists such as J. de Arfe Villafañe (1535-1603), D. de Santiago, and Á. Alonso Barba (1569-1662), the author of 'Arte de los metales'. He developed the method for recovering silver and gold by using mercury extracted in Almadén (La Mancha), the largest mercury mine in the world. In addition, America and the Far East provided stunning and fascinating mineral samples for collectors and scientists of the New World. The Spanish Royal Cabinet of Natural History was created in 1771 from the collection of minerals of P. Franco Dávila (1711-1786). It was probably the best collection of its time, and was used by R. de L'Isle (1736-1790) during his studies on crystal morphology.

The first Spanish scientific journal, printed in 1799 included articles on the nature of crystals by mineralogists educated in the Wernerian School of Freiburg. The controversy between Werner's ideas on the classification of minerals based on external properties and the new concept introduced by R. de L'Isle and the abate René Just Haüy (1743-1822) on crystal morphology is clearly observed in the 'Anales de Historia Natural'. It demonstrates how aware Spanish scientists were of the crucial changes occurring in mineralogy during the 18th and 19th centuries.



Some crystallographic models of the abate Haüy.

A collection of crystallographic solids given by Haüy to the Galician mathematician J. Rodríguez González (1770-1824) was used by crystallographers G. de Linares (1845-1904) and L. Calderón (1847-1894) who established what was probably the first (1888) Chair of Crystallography in a European University.



Francisco Pardillo (1884-1955) (Photo courtesy of the Royal Acad. of Sciences and Arts of Barcelona).



Left: Blas Cabrera (1878-1945). Middle: Gabriel Cardoso (1896-1954). Right: Julio Palacios (1891-1970).



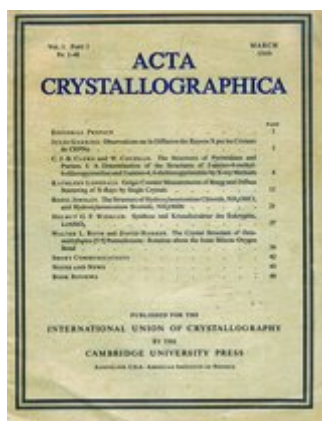
Top: The National Institute of Physics and Chemistry (Instituto Nacional de Física y Química, Madrid, 1932). It was named 'The Rockefeller' due to the fact that it was built using funds (\$200 000) from the Rockefeller Junior Foundation. Bottom: 'The Rockefeller' today, as Institute of Physical Chemistry 'Rocasolano', is one of the research Institutes of the CSIC, the Spanish National Research Council.

At the beginning of the 20th century, the Spanish crystallographer F. Pardillo immediately recognized the importance of the investigations of Laue and Bragg. In 1923 he reported these studies to the Boletín de la Real Sociedad Española de Historia Natural. Two years later, B. Cabrera (who later became director of the Instituto Nacional de Física y Química) wrote a report on the novel application of X-rays to determine the structure of materials in the 'Anales de la Sociedad Española de Física y Química'.

G. M. Cardoso (Museo Nacional de Ciencias Naturales, Madrid), J. Palacios (Instituto Nacional de Física y Química) and Francisco Pardillo (Dept. of Mineralogy of Barcelona) formed the first Spanish groups of modern crystallography. L. Rivoir worked with Palacios on structure determinations of inorganic and organic crystals and on the perfection of the Fourier methods of analysis. Pardillo created a crystallography school at the U. Barcelona.



Left: Luis Brú (1909-1997). Middle: José L. Amorós (1920-2001). Right: Julio Garrido Mareca (1911-1982). After the Spanish Civil War, young crystallographers created the foundations of current Spanish crystallography. L. Bru advanced X-ray and electron microscopy first in the Canary Islands, later in Sevilla and finally at the U. of Madrid. L. Rivoir headed the X-ray Dept. at the Instituto de Física, Consejo Superior de Investigaciones Científicas (CSIC), the Spanish National Research Council, and J. L. Amorós formed a group of young crystallographers and crystal growers at the U. of Madrid.



The first volume of Acta Crystallographica (1948) contained an article by J. Garrido on 'Observations sur la diffusion des rayons X par les cristaux de NaClO_3 ' and a review of the book by J. Garrido and J. Orland 'Los rayos X y la estructura fina de los cristales: Fundamentos teóricos y Métodos prácticos' (1946). The Spanish National Crystallographic Committee (founded by CSIC) joined the International Union of Crystallography in 1949.

In 1950, a Spanish Association of Crystallography (ACE) of 35 members held its first meeting in Barcelona. Ten years later the Ibero-American Association for Crystallography was founded.



Left: M. Font-Altaba (1922-2005). Middle: S. García-Blanco (1922-2003). Right: S. Martínez-Carrera (1925-).

At that time there were two main schools of crystallography in Spain, those of M. Font-Altaba (U. of Barcelona) and S. Martínez-Carrera and S. García-Blanco (CSIC). S. Martínez-Carrera brought experience gained in Pittsburgh with computing programs that replaced the Beevers-Lipson strips. These groups used Weissenberg cameras and the first IBM computers. In the 70s, four-circle single-crystal diffractometers replaced Weissenberg and precession cameras.



Left: Weissenberg cameras and X-ray tubes used in Madrid during the 60s. Right: The first automated 4-circle diffractometer (PW1100) installed in Spain, Madrid, in 1973.

The 'Rocasolano' (CSIC) group in Madrid strengthened the crystallographic community in all of Spain by collecting data, and creating and maintaining the first crystallographic software collections in Spain (installed on a UNIVAC mainframe). They also negotiated with the Cambridge Crystallographic Data Centre (CCDC) for distribution of the CSD crystallographic database throughout the country. Thanks to the generosity of the CCDC, this agreement later covered all Latin American countries as well.



J. M. Bijvoet and his wife (Madrid, 1956).

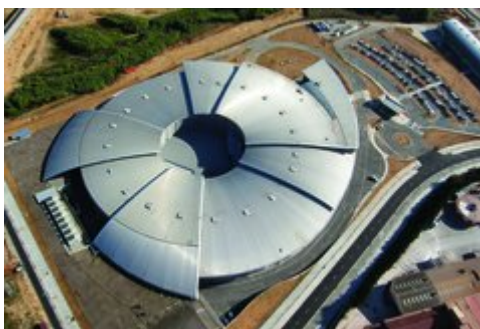


The first Inter-Congress meeting of the IUCr, held in Madrid in 1956.



From left to right: L. O. Brockway and wife, and Gunnar Hägg (Madrid, 1956).

The importance of crystallography for the development of chemistry in Spain led to the growth of several crystallographic groups. In this enterprise a generation of young Spanish crystallographers born around 1940 played an important role, elevating Spanish crystallography to its rightful place on the international stage. Many of them have passed away, including F. H. Cano (CSIC) and X. Solans (U. of Barcelona), others have retired, such as J. Fayos and Francisco Sanz (CSIC) and J. A. Subirana (Polytechnic U. of Barcelona), while others are still active, including Carlos Miravittles, C. Foces-Foces, E. Iglesias, M. Martínez-Ripoll (CSIC) and J. M. Amigó (U. of Valencia). However, crystallography in Spain, and especially in academic institutions, still seems to be erroneously considered a minor technical skill, whose application and interpretation is trivial. Despite the importance of crystallography for biology and biomedicine, and the rather large number of research groups in Spain in cellular and molecular biology, the lack of resources dedicated to macromolecular crystallography is very apparent. At the end of the eighties Spain became the first associate scientific member of the Institute Laue-Langevin (ILL), the high-flux neutron reactor of Grenoble, and new possibilities were opened for the crystallographic community including physicists, biologists and engineers. Increased activity developed around magnetic crystallography, soft condensed matter, liquids and amorphous systems, and biology. Synchrotron techniques for crystallographic studies brought Spanish crystallographers to the European Synchrotron Radiation Facility (ESRF).



View of the Spanish synchrotron ALBA as in November 2009.

Today the Spanish Group on Crystallography and Crystal Growth (Grupo Especializado de Cristalografía y Crecimiento Cristalino, GE3C) has over 200 members. If other crystallographers associated with neutron, solid state, proteomics and surface applications are taken into account, then about 400 Spanish researchers are currently involved in crystallographic research. Most Spanish crystallographers are organized in teams in the Canary Islands, Andalusia, Valencia, Asturias, Catalonia, Galicia, the Basque Country and Madrid, as well as others. They share over 200 X-ray diffraction machines for both powder and single-crystal applications, and maintain active participation in neutron and synchrotron techniques in different European facilities (the ILL and the ESRF). The Spanish synchrotron ALBA was inaugurated in March 2010 with several crystallographic beam lines. Electron microscopy will also be well represented there, from high-resolution transmission electron microscopy to field emission electron scanning microscopy.



Meeting on Anomalous Scattering, held in Madrid in 1974.



From left to right, Dorothy Hodgkin, S. C. Abrahams and S. Martínez-Carrera (Madrid, 1974).

Spanish crystallographers hold a yearly national congress and have also organized several international seminars, workshops, conferences and meetings. At the Executive Committee meeting arranged during the Third General Assembly in Paris in July 1954, it was proposed that the IUCr should organize specialized symposia between the assemblies. The first of these meetings was held in Madrid in 1956 and since then, specialized Inter-Congress meetings have become a regular feature of the Union's activities. In April 1974 an Inter-Congress Conference was held in Madrid on the subject of anomalous scattering, the results of which were assembled into a valuable book dealing with every conceivable aspect of anomalous scattering known at that time.

Thanks to the explicit votes of Mario Nardelli (Italy) and Olga Kennard (UK), as well as to the financial support given by M. Font-Altaba (the Mayor of Barcelona), the 6th European Crystallographic Meeting (ECM-6) was successfully held in Barcelona during the summer of 1980, with Carlos Miravittles as Chairman.

Now, nearly one hundred years since Laue and Bragg's experiments, we are preparing to host the XXII Congress and General Assembly of the International Union of Crystallography (www.iucr2011madrid.es/) in Madrid. It will be a spectacular and memorable event from both scientific and social perspectives (see later in this issue for more information on the Congress).

Next Issue... 'Crystallographers in Spain'.

M. Martinez-Ripoll

MEETING REPORT

12th Heart of Europe meeting

Třešť', Czech Republic, September 2009, www.img.cas.cz/hec/



Participants at the 12th Heart of Europe Bio-Crystallography Meeting.

One hundred and seven participants gathered this year in Třešť' (Czech Republic) on September 24-26 for the 12th Heart of Europe bio-Crystallography Meeting. In good tradition since 1998, mainly PhD students presented their results (and problems) in a total of 27 talks. The meeting was held in the Castle Hotel Třešť', which provided an elegant atmosphere for the talks and breaks. Most participants were accommodated in the building, which was transformed from a fortress into a castle during the 15th century. Pavlína Řezáčová and her structural biology group from Prague organized a stimulating scientific meeting and a pleasant stay for the participants.

A highlight of the meeting is traditionally the invited HEC lecturer, which this year was given by Paul Emsley (U. of Oxford). In a vivid and diverting talk, Paul reported about the development of the *Coot* program and provided insight into its many helpful functions for crystallographic model building. For the free time on Friday afternoon a trip to Telc was organised. The town was founded in the 13th century as a royal water fort on the crossroads of busy merchant routes between Bohemia, Moravia and Austria and is now a UNESCO World Heritage Site.

A prize for the best presentation was sponsored by the IUCr: the book 'Crystallography across the sciences'. This year the prize was awarded to two participants: P. Mader (IMG, Prague) and E. Ch. Schulz (U. of Göttingen). A bar of the favorite Czech chocolate 'Studentska pecet' (Student's seal) was awarded for the best pronunciation of the name Třešť'. L. Schulz (EMBL Hamburg) was also rewarded with this chocolate for her active participation in the discussion after the talks. The HEC organizers hope for a stronger participation of the PhD students in the discussions in the future. Altogether, HEC-12 presented another highlight in the long history of the HEC-meetings. All of the participants enjoyed exciting lectures, made plenty of new friends, and, last but not least, look forward to HEC-13, which will be organized by Norbert Sträter and his group in the lovely town of Schöneck in September 2010.

Norbert Straeter

MEETING REPORT

Neutrons in Biology conference

Santa Fe, NM, USA, October 2009

The International Conference on Neutrons in Biology was held in Santa Fe in October 2009 to review recent progress and to celebrate Benno Schoenborn's many contributions to the field. Following a very distinguished career in national research laboratories and universities around the world, Benno formally retired from LANL in May 2009, however he will continue as Senior Fellow at LANL and Professor at the U. of Sydney.

Neutron protein crystallography is a powerful technique to investigate mechanisms of enzyme activity, inhibitor binding *etc.* where details of H positions, particularly in the vicinity of the active and/or recognition sites, lead to a better understanding of molecular interactions. Ryota Kuroki (JAEA) presented two examples of drug binding to receptors - porcine pancreatic elastase (PPE) with potent inhibitor FR13080, and human immunodeficiency virus type-1 protease (HIV-PR) with potent inhibitor KNI-272. Julian Chen (Goethe U.) is determining the structure of diisopropyl fluorophosphatase (DFPase), a calcium-dependent phosphotriesterase, in order to better understand its ability to detoxify a wide range of organophosphorous nerve agents. Investigations into the molecular mechanism(s) of sweet taste were presented by Susana Teixeira (Keele U., ILL) using the structure determination of the artificial sweetener, thaumatin. Andrey Kovalevsky (LANL) presented the findings of a very elegant study on the Bohr effect in the allosteric binding and release of oxygen in Hb. Carbonic anhydrase is a ubiquitous metalloenzyme that reversibly converts carbon dioxide to carbonic acid and bicarbonate ions in the mammalian respiratory system. Zoë Fisher (LANL) described the latest results of studies on the hydrated proton-transfer wire implicated in the enzymatic process. Jenny Glusker (Fox Chase Cancer Centre) illustrated recent work on the movement of H atoms involved in sugar conversion by *D*-xylose isomerase - an important enzyme for biofuel production.

Studies of the phase transitions, hydration, folding/unfolding and drug binding in DNA using complementary X-ray and neutron scattering and diffraction techniques was presented by Trevor Forsyth (Keele U., ILL). Developments in experimental techniques were highlighted and recent results presented.

Progress toward developing a unified model for protein dynamics was presented by Hans Frauenfelder (LANL). Such a model requires a good understanding of backbone motions as well as interactions with individual solvent molecules and the bulk. Fluctuations in the hydration shells and bulk solvent have a significant influence on protein structure and dynamics.

Recent developments in instrumentation for neutron protein crystallography stressed the importance of small crystal size ($\sim 0.1\text{--}0.2\text{ mm}^3$), macromolecular deuteration, increased neutron flux, more and larger area detectors, and increasingly sophisticated software for data processing and analysis. The features and performance were presented for iBIX at JPARC (Ichiro Tanaka, Ibaraki U.); LADI-III at the ILL (Matthew Blakeley, ILL); TOPAZ at the SNS (Xiaoping Wang, ORNL), and PCS at LANSCE (Andrey Kovalevsky, LANL).

A highlight of the conference was a mini-symposium on 'Neutrons for Renewable Energy and the Environment'. Various aspects of this priority field of research were presented, from detailed studies of the hydrogen-bonding network in cellulose fibres (Yoshi Nishiyama, CNRS) to the complex multi-component cellulosic biomass structures including longer length scales (Paul Langan, LANL). Looking for a better understanding of enzymatic and/or chemical processing of cellulose fibres, Mike Kent (SNL) used the SANS technique to monitor enzymatic digestion *in situ*, and Venki Pingali (ORNL) explored the structural effects of acid pre-treatment. Molecular modelling of the hydrogen-bonding network in cellulose fibres was reported by Gananakaran (LANL).

The *PHENIX* (www.phenix-online.org) and *nCNS* (mnc.lanl.gov) software packages are being developed for the international neutron macromolecular crystallography community by an NIH-funded consortium of scientists led by Paul Langan (LANL) and Paul Adams (LBL). These packages now include a new generalized X-ray and neutron crystallographic analysis approach that provides more accurate and complete structures for biological macromolecules. Pavel Afonine (LBL) presented an excellent overview, and then together with Marat Mustyakimov (LANL) led a workshop on 'Computational Tools in Neutron Crystallography' in which informal discussions and hands-on tutorials demonstrated the many features of both packages.

Small-angle neutron scattering (SANS) is a valuable technique to investigate structure on longer length scales. William Heller (ORNL) described the dedicated Bio-SANS instrument at HFIR and Cameron Nylon (STFC) described the new SANS2d instrument at ISIS, which is an example of the next generation of SANS instruments with two tandem 2D detectors. Rex Hjelm (LANL) presented the findings of a fascinating study using SANS to unravel the complex dynamic process of moving cellular organelles along the microtubule network.

Neutron reflectivity is used extensively to study the structure of biological membranes. Jarek Majewski (LANL) used a thermo-responsive polymer to tailor the local curvature of a fully hydrated tethered bilayer, thus forming an excellent model for an intact biological membrane. Luke Clifton (U. of Reading) explored the interaction of puroindolines - seed defense proteins in wheat - with lipid bilayers to better understand wheat endosperm texture, and also provide valuable insight into protein-lipid interactions.



Dean Cole from the Office of Biological and Environment Research of the US Department of Energy presenting Benno with a letter from DOE headquarters thanking Benno for his service. The letter is being held by Alan Hurd, the Director of the Manuel Lujan Neutron Science Center at Los Alamos National Laboratory.

Benno Schoenborn was the distinguished after-dinner speaker and entertained guests with the 'History of Neutrons in Biology'. This was a colourful narrative of the development of the unique contribution of neutron scattering applied to biological structures. There were numerous anecdotes. Benno first discussed the possibility of neutron diffraction to investigate H bonding in proteins with Herman Watson, Uli Arndt, John Kendrew and Christopher Nobbs in the MRC tearoom in 1965. As usual, Benno was of the view that just because something was considered to be almost impossible did not mean it could not be done. Two years later, with support from Christophe Hirs and using Walter Hamilton's single-detector diffractometer at HFBR (BNL), Benno collected the first diffraction peaks from a rather large (by today's standards) myoglobin crystal. It took almost a year to collect a complete dataset and the results were published in *Nature* in 1969. Benno's career is a kaleidoscope of people, places and achievements, always pushing the limit in knowledge, theory, instrumentation and software, the impact of which will be substantial well into the future. Throughout his career Benno supervised and encouraged a generation of students and Early Career Scientists, and is an inspiration and mentor to many.

The organizers are grateful for financial support from Materials Research Society, the Office of Biological and Environmental Research of the US Department of Energy, and the Los Alamos National Laboratory. The proceedings of the conference will be published in a special issue of *Acta Crystallographica*.

Paul Langan (Conference Chair) and Robert Knott

MEETING REPORT

ISDSB2010

Orsay, France, May, 2010. www.synchrotron-soleil.fr/Workshops/2010/ISDSB/



Professor Roger Fourme opens ISDSB2010.



The ISDSB2010 conference dinner on a Parisian River Seine cruise boat.

The 3rd International Symposium on Diffraction Structural Biology (ISDSB2010) was held at Paris-Sud U. and the nearby national synchrotron radiation facility SOLEIL, the first to be held outside Japan. The ISDSBs were begun in 2003 by the Japanese Society for the Promotion of Science (JSPS), and the University-Industry Cooperative Research Committee chaired by Noriyoshi Sakabe.

The ISDSB Symposia bring researchers who use X-ray, electron and neutron diffraction techniques to study structural biology together with scientists who use microscopies and spectroscopies (in particular NMR) to study biological ultra-structure. The symposia foster a more systematic understanding of biological function. The scientific topics covered in ISDSB2010 included electron microscopy, X-ray imaging, tomography, drug and vaccine design, protonation states, membrane proteins, protein structure and function, X-ray technologies, and structural genomics. The symposium provided a comprehensive overview of the latest achievements and trends. A total of 201 participants from 18 countries took part. The speakers included 2010 Nobel Prize winner, Venki Ramakrishnan, six plenary lecturers (Wolfgang Baumeister, Tom Blundell, Gérard Bricogne, Wayne Hendrickson, Claudio Luchinat, Dmitri Svergun and Ichiro Tanaka) and twenty six other invited speakers. There were poster sessions, a commercial exhibition and as a visit to the SOLEIL facility. The conference papers are to be published in the *Journal of Synchrotron Radiation* (Nori Yasuoka, Guest Editor). Student attendance was supported by

the European Crystallographic Association (ECA) and the IUCr. At a 'Meet the public' event hosted by the Director General of SOLEIL, M. van der Rest, a panel comprised of the plenary speakers addressed the importance of basic science and major regional facilities such as synchrotron and neutron sources, including the new Japanese JPARC spallation neutron source. Questions addressed by the panel included the image problem that science has with the public, the need to respond promptly to disease challenges, and why there is a time lag between basic science breakthroughs and their applications. The conference closed with an invitation from Japan to host the 4th ISDSB in May 2013.

ISDSB2010 Organizers Roger Fourme, John R. Helliwell, Jack Johnson, Noriyoshi Sakabe and Noritake Yasuoka

MEETING REPORT

High-Pressure Single-Crystal Diffraction Workshop

Poznań, Poland, April, 2010



Participants of the 3rd Frolic Goats High-Pressure Workshop in Poznań (left to right): Andrzej Katrusiak, Marek Szafranski, Maciej Hodorowicz, Michał Andrzejewski, Roman Minikayev, Kamil Dziubek, Marek Daszkiewicz, Maciej Bujak, Julia Bąkiewicz, Anna Olejniczak, Marcin Podsiadło, Olga Ermakova, Ewa Werner-Malento, Paulina Małecka, Klaus Merz, Julia Skumiel, Paweł Piszora, Vera Vasylyeva, Marcin Jarek, Teresa Kubacka and Wojciech Nitek.

The 3rd Frolic Goats High-Pressure Diffraction Workshop, held at the Adam Mickiewicz U., April 26-27, 2010, was attended by 30 crystallographers. This 'organic work' type of conference is aimed mainly at disseminating single-crystal high-pressure diffraction techniques used in crystallographic laboratories and at consolidating the high-pressure crystallographic community in the region. The audience included both beginner and expert high-pressure crystallographers. A series of lectures on high-pressure studies with conventional four-circle diffractometers, synchrotron and neutron sources and high-pressure data reduction were followed by application of pressure to specific subjects of crystal chemistry and materials sciences (Andrzej Katrusiak, Klaus Merz, Marek Szafranski, Maciej Bujak, Marcin Podsiadło, Kamil Dziubek, Damian Jęczmiński, Michał Andrzejewski, Julia Bąkiewicz, Marek Daszkiewicz and Marcin Jarek). There were vivid discussions and afternoon laboratories on assembling high-pressure equipment, loading diamond-anvil cells, centering it on a CCD diffractometer, data collection and processing. High-pressure research at the Faculty of Chemistry, Adam Mickiewicz U., is currently financed by a TEAM grant from the Polish Foundation of Science. In the evenings participants enjoyed the historical first capital of Poland, in the heat of Polish Football Extra-league finals, eventually won by Poznań team Lech and decently celebrated on May 15.

Andrzej Katrusiak

BOOK REVIEW

Robert Olby on Francis Crick (1916-2004)

The discovery of the double helix by Watson and Crick in 1953 must be the most widely reported molecular structure determination of the 20th century. In 1951, with a passion for DNA and a background of ornithology, genetics and phages, Watson went to Cambridge, England, where Crick taught him some crystallography. Prior to 1949, Crick had been a physics research student in London, a Royal Navy scientist, and then a researcher in cell biology at the Strangeways Laboratory near Cambridge. In 1949 he joined Max Perutz at the new Medical Research Council Research Unit in Molecular Biology at Cambridge. In addition to intellect, energy, enthusiasm and verbosity, Crick had an immense power of concentration when reading scientific books and papers. Indeed, he wrote that, while the double helix would doubtless have been discovered by others within a year or two, what Watson and he should be credited with was for taking the trouble to learn about X-ray crystallography as well as other diverse topics. Much of Crick's achievement derived from incessant intellectual argument with, in turn over the decades, three brilliant, appreciably younger, international collaborators including the American James Watson, author of *The Double Helix*, the tone of which Crick did not like. His longest collaboration was at the MRC Unit in Cambridge with Sydney Brenner, of Lithuanian extraction but brought up in South Africa. In his later years, Crick communicated about consciousness with Christof Koch, whose early life had been in Europe, North Africa, and North America.

In 2006, the science writer Matt Ridley published a short authoritative and very readable biography of Crick without references or index. Robert Olby, a science historian, first encountered Crick in 1966 and, with Crick's encouragement, has written in the past about Crick and the path to the double helix, as well as composing biographies of many of the associated scientists. He has now produced a full authoritative scholarly biography, *Francis Crick: Hunter of Life's Secrets* (Cold Spring Harbor Press, 2009), with index, notes of sources, timeline, biographical sketches of many of the scientists involved, and an excellent collection of photographs. Olby describes Crick's comfortable home background and education in England and how a brilliant scientist emerges from what had seemed a merely rather clever one. He relates both the pre-crystallographic life of Crick and the later years on neuroscience at the Salk Institute in the USA. This biography, by an author knowledgeable about the history of molecular biology, describes the life of a Nobel prizewinner whose passion for the science between the living and the non-living took him into embryology, neuroscience and the study of consciousness. It is highly recommended, but those with more limited time or less interest should not ignore Ridley's briefer life story, which is perhaps rather better on the personal side.

Derry W. Jones

Editors' note: For additional views on the history of the discovery of the double helix see 'Rosalind Franklin and DNA' by Anne Sayre and/or 'Rosalind Franklin: The Dark Lady of DNA' by Brenda Maddox.

OBITUARY

Clara Brink Shoemaker (1921-2009)



Clara Brink Shoemaker, professor emeritus at Oregon State U., died September 30, 2009. Clara was born in Rolde, Netherlands, in 1921. She received her doctorate in chemical crystallography from Utrecht U. in 1950, having studied crystallography with Caroline MacGillavry in Amsterdam, with whom she published the crystal structures of K_2AgI_3 and K_2CuCl_3 . Clara worked with Dorothy Hodgkin on Vitamin B12 in Oxford and was encouraged, both by MacGillavry and Hodgkin, to consider further postdoctoral experience. Possibly influenced by a niece living in Boston who was married to Nicolaas Bloembergen, a faculty member in Harvard's Physics Department and subsequent Nobel Prize winner, she went to MIT, where she was warmly welcomed by Martin Buerger and Bertram Warren.

Her collaboration with David Shoemaker led to their first joint study published in *Acta Cryst.* in 1955. They established the σ -phase materials as typifying a promising new field. In August of that year, Clara and David were married in MIT's chapel. They were the first to recognize that interstices in tetrahedrally close-packed metal crystals are exclusively tetrahedral, with coordination types restricted to a set of four with coordination numbers 16, 15, 14 and 12. They also noted that half the hexagonal holes present in σ -phase materials become distorted pentagons in the P -phase, resulting in a coordination number reduction from 14 to 12 in half the atoms of the subsidiary layers.

Many contributions to this new field of intermetallic structure followed, including a major paper by Linus Pauling in 1988 on icosahedral cluster P -phase packing that acknowledged their early work. Among these are numerous X-ray and neutron diffraction and modeling studies by others. The σ and P phases, now among the most intensively studied intermetallics due to their tendency to precipitate from stainless steels in the form of austenitic, ferritic or austenitic-ferritic phases, have given rise to a large literature in which the pioneering work of Clara and David is often referenced.

Clara's breadth of interest is exemplified by her publications, including an insulin analysis with Barbara Low, the nature of the S-O bond with Klass Eriks, a coding system applicable to a wide range of layered tetrahedrally close-packed structures, a hypothetical tetrahedrally close-packed σ -phase proposed by Erwin Parthé, and demonstration of the existence of the pentagon- σ structure with composition FeSiW with Bill Pearson, NRC Canada.

In 1970, David accepted both the chairmanship of the Chemistry Department at Oregon State U. and the presidency of the American Crystallographic Association. State regulations prohibited close family members from holding faculty positions at the same time. The potential impediment to Clara's appointment was examined by the president of the university, Robert MacVicar, who discovered that the law prohibited joint family appointments 'except under exceptional circumstances'. He announced that any husband and wife scientific team qualified as an exceptional circumstance and Clara's appointment, as well as that of Lise Hedberg, wife of one of the present authors, went forward. It was determined that each husband would take responsibility for the scientific effort of the other's wife. This arrangement required that each husband assure the other that his wife was doing a good job. The process was certainly easy to carry out, but seems a bit comical in retrospect. Clara and David attended all IUCr Congresses from the 4th (Montreal, 1957) to the 13th (Hamburg, 1984).

Clara maintained her departmental contacts after David's death, joining a luncheon discussion group each Friday and participating in morning coffee-break sessions. She enjoyed both chamber and orchestral music and regularly attended the Oregon Shakespeare Festival.

Erudite and cultured, Clara was also kind, gentle and characteristically reserved. She loved her family and was proud of her son Robert, Professor of 18th-Century British History and Co-Director, Old Bailey Online, Plebeian Lives and the Making of Modern London, at the U. of Sheffield in the UK. She was delighted that her grandson Roland is presently a third-generation Shoemaker undergraduate at Reed College. Clara Brink Shoemaker was a fine person in every respect, and her friends and colleagues will miss her greatly.

We gratefully acknowledge the biographical notes on Clara compiled by Mary F. Singleton, available at: osulibrary.oregonstate.edu/specialcollections/coll/shoemaker/singleton/page1.html

Sidney C. Abrahams and Kenneth Hedberg

OBITUARY

Yoshio Takéuchi (1924-2009)



Yoshio Takéuchi, Emeritus Professor of the U. of Tokyo, passed away at the age of 85 on July 5, 2009 in Tokyo, Japan. He was born in Tokyo on Jan. 20, 1924 and educated at the U. of Tokyo. During his PhD course he studied crystal structures of mineral polymorphs with T. Ito and R. Sadanaga, where his idea on the symmetry elements gliding of unit-cell twinned space groups contributed to the publication of *X-ray Study on Polymorphism* (T. Ito, Maruzen, 1950). In 1952 he went to M. J. Buerger's laboratory at MIT to determine the crystal structure of terramycin hydrochloride by using vector sets in Patterson space (*Proc. Natl Acad. Sci.* **46**, 1366, 1960). Leaving for home in 1956, he was consecutively lecturer, associate professor and professor of the Mineralogical Institute at the U. of Tokyo. After his retirement in 1984, he moved to Nihon University to teach students mineralogy and crystallography until 1998.

He was a member of the IUCr Commission on Crystallographic Computing in 1960s, a co-editor of *Zeitschrift für Kristallographie* and a member and secretary of the Japanese National Committee for Crystallography until the 1980s. He served on various international bodies such as the Joint Committee on Powder Diffraction Standards (JCPDS) and the International Centre for Diffraction Data (ICDD). He was active in Japan, serving as a president of the Crystallographic Society of Japan as well as the Mineralogical Society of Japan. He contributed to organizing the IUCr72 Kyoto Congress and the establishment of the Photon Factory synchrotron facility and large-scale computing centers among universities.

He published numerous research papers, in which his main and deep interest was made up into a book of *Tropochemical Cell-Twinning (A Structure-Building Mechanism in Crystalline Solids)*, published in 1997 by Terra Scientific Publishing Co., Tokyo. The free pdf files are available on the website www.terrapub.co.jp/e-library/tct/index.html. In 1978 he introduced the concept of tropochemical cell-twinning (TCT) as a crystallographic mechanism of building complex structures. The TCT mechanism with crystallographic slips can characterize the crystal structure and crystal chemistry of the homologous series and non-stoichiometric compounds.

He was always a kind, enthusiastic and open-minded gentleman with a gift for finding younger research scientists. He was interested in serendipity and recently engaged in the editing and Japanese translation of the fairy tale of *The Three Princes of Serendip*. His many friends mourn his passing.

Satoshi Sasaki

OBITUARY

Lodovico Riva Di Sanseverino (1939-2010)

Lodovico with Carlo Mealli and Paola Paoli at the Florence Congress in 2005, where he received an award for Award for Exceptional Service to Crystallography for his organization of the Erice Schools.

Lodovico Riva Di Sanseverino passed away on 18 June 2010 at the age of 70. Lodovico was Professor of Chemistry and Mineralogy at the U. of Bologna and since 1974 had been the organizer of the International School of Crystallography in Erice. He was born in Palermo in 1939 and, after starting his chemistry career at the U. of Palermo, he graduated from the U. of Florence in 1962. After some periods spent in The Netherlands and in England, he pursued his scientific career as full Professor at the U. of Bologna, starting in 1975.

He died unexpectedly in hospital in Sicily a few days after closing the latest course of the Crystallographic Schools in Erice, which, also thanks to the invaluable collaboration with Paola Spadon, was the usual outstanding success. To underline the height reached by this 42nd course entitled 'Structure and Function from Macromolecular Crystallography: Organization in Space and Time' (directed by T. L. Blundell and M. A. Carrondo), as many as three Nobel Laureates had gladly accepted to be teachers.

Lodovico had decided not to return immediately to Bologna after the school, but to stay in Erice, because his support could be helpful to the next course, once again related to crystallography, namely 'Structural and Molecular Archaeology', directed by G. Tsoucaris.

We wish to remember Lodovico with the contented expression of the present photo, which was taken during the banquet of the XX IUCr Congress in Florence in 2005, when the Union presented him with an Award for Exceptional Service to Crystallography for his organization of the Erice Schools.

Lodovico leaves behind his wife Fiorbellina, his son Clemente, his daughter Claudia and two grandchildren.

Carlo Mealli

IUCR ACTIVITIES

Save the date for Madrid 2011

Madrid, Spain, August 22-30, 2011. www.iucr2011madrid.es



The Alcala gate: an emblematic monument of Madrid.



A night image of the Alhambra in Granada: a clear exponent of Spanish culture.

By the time you read these lines there will be less than one year until the next Congress and General Assembly of the IUCr. It is time to put the dates on your calendar and plan to be in Madrid to hear about the latest developments in Crystallography and to get a feeling for the Spanish way of life.

It has been a long time since a group of Spanish crystallographers started to prepare the proposal to host the IUCr meeting in Spain and work has continued since the time that the bid was successful. In the past two years, we have been working hard to assure perfect organization of the Congress. We have invited the best scientists working in the different areas of crystallography to participate in the meeting and we will offer excellent opportunities to explore our country.

The second circular for the Congress will be in the next issue of the IUCr Newsletter (Vol. 18, No. 4). It will provide all the details for the Madrid meeting: information concerning invited speakers, microsymbiosia topics and all parallel activities that will be running during the conference. Additionally, we are organizing a number of attractive satellite events (schools, workshops, etc.) that will offer you the possibility of visiting other places that show off the fascinating geography of Spain.

It is clear to all of us that an international scientific meeting offers not only a unique opportunity to get the latest research advances directly from those carrying out these exceptional investigations but also the opportunity to interact first hand with the traditions and lifestyle of the country we visit. Spain is the perfect place to get a flavor of Mediterranean culture and of the origins of civilization in Europe. For these and many other reasons, be sure and mark your calendar to be with us for the next IUCr meeting in Spain in August 2011. You can also find all the information about the Congress on our website. We hope to see you in Madrid!

Martín Martínez-Ripoll and Fernando J. Lahoz