INTERNATIONAL UNION OF CRYSTALLOGRAPHY

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Original article text and available illustrations

Contents

> Extraction incomplete: missing article positions 1.

IUCr journals news

Disputed discovery: the beginnings of X-ray diffraction in crystals in 1912 and its repercussions 3

Structure maps for AI4AII6(BO4)6X2 apatites via data mining 4

1-Ferrocenylmethyl-3-(2,4,6-trimethylbenzyl)-1H-imidazolidin-3-ium iodide and trans-bis(3-benzyl-1-ferrocenylmethyl-1H-imidazolidin-2-ylidene)diiodidopalladium(II) 5

Rapid visualization of hydrogen positions in protein neutron crystallographic structures 6

(3R,4S,5S,8S,10R,13R)-3-Hydroxykaura-9(11),16-dien-18-oic acid 7

Structure of CBM3b of the major cellulosomal scaffoldin subunit ScaA from Acetivibrio cellulolyticus 8

Quantification of passivation layer growth in inert anodes for molten salt electrochemistry by in situ energy-dispersive diffraction 9

Increase of lifespan for glioma-bearing rats by using minibeam radiation therapy 10

Meeting report

XXII IUCr Congress and General Assembly 11

Erice Schools of Crystallography 29

8th International School on Crystallography and X-ray Diffraction 33

Awards and prizes

The 2011 Gregori Aminoff Prize in Crystallography goes to Addadi and Weiner 26

Brunger wins inaugural DeLano Award 27

Notice

Acta C publishes virtual issues on polymorphism and absolute structure 28

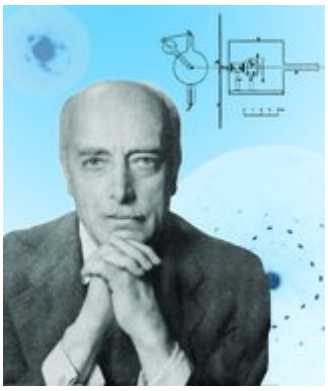
Obituary

Gabriel Germain (1933-2011) 34

IUCR JOURNALS NEWS

Disputed discovery: the beginnings of X-ray diffraction in crystals in 1912 and its repercussions

Acta Cryst. (2012). 68, 30–39 (http://doi.org/dnvfnj)



Max von Laue (1879–1960) with diffraction patterns obtained from crystals of copper sulfate (top left) and zinc blende (bottom right), and the experimental setup used [W. Friedrich, P. Knipping & M. Laue (1912). *Sitzungsber. K. Bayer. Akad. Wiss.* pp. 303–322].

The discovery of X-ray diffraction by crystals in 1912 was motivated by misapprehensions. Max von Laue expected an interference of characteristic X-rays emitted by the crystal atoms. The ensuing experiments by W. H. and W. L. Bragg clarified the phenomenon, although they too started from erroneous assumptions about the nature of X-rays. The discovery and its application for X-ray crystallography received a swift recognition by the Nobel awards to Laue and the Braggs in 1914 and 1915, respectively, but the circumstances of the discovery remained the subject of dispute.

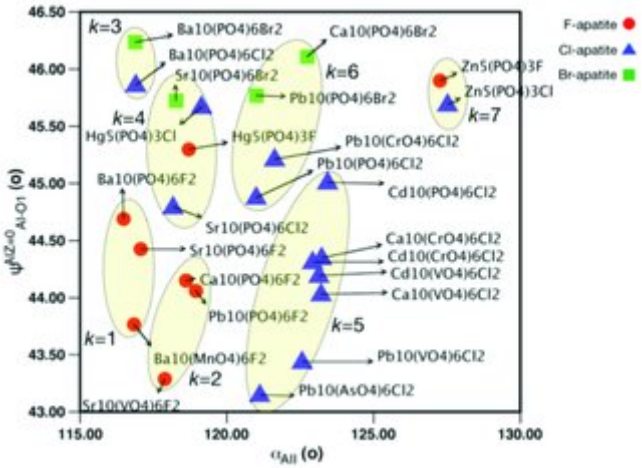
M. Eckert

IUCR JOURNALS NEWS

Structure maps for AI4AII6(BO4)6X2 apatites via data mining

Structure maps for $A^{I}_{4}A^{II}_{6}(BO_4)_6X_2$ apatites via data mining

Acta Cryst. (2012). B68, 24–33



A new structure map for apatites defined using the two key bond distortion angles α_{All} and $\Psi_{Al\text{-}O1}^{Alz\text{-}0}$. The paper describes a novel approach based solely on data mining methods to discover crystallographic relationships that provide new classification patterns in complex apatite structures associated with site occupancy. This work shows how new structure maps for classification of crystal chemistries can be developed without any *a priori* assumption of what factors govern that classification, and in the process uncover new and unexpected chemistry–structure relationships. More generically this study provides a template for a data driven, 'genomic' style strategy for materials design and discovery.

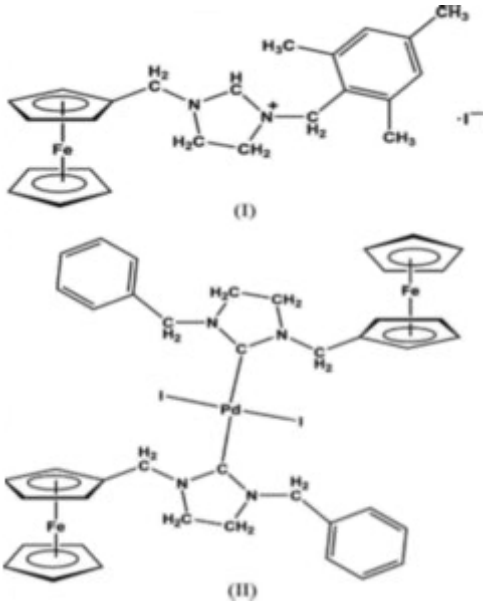
P. V. Balachandran and K. Rajan

IUCR JOURNALS NEWS

1-Ferrocenylmethyl-3-(2,4,6-trimethylbenzyl)-1H-imidazolidin-3-ium iodide and trans-bis(3-benzyl-1-ferrocenylmethyl-1H-imidazolidin-2-ylidene)diiodidopalladium(II)

1-Ferrocenylmethyl-3-(2,4,6-trimethylbenzyl)-1*H*-imidazolidin-3-ium iodide and trans-bis(3-benzyl-1-ferrocenylmethyl-1*H*-imidazolidin-2-ylidene)diiodidopalladium(II)

Acta Cryst. (2012). C68, m48–m52 (http://doi.org/fxzh8t)



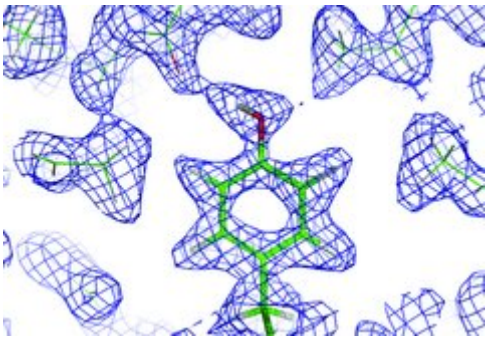
N-Heterocyclic carbenes are compatible with most transition metals and generally lead to air-stable and thermally robust complexes that do not undergo ligand dissociation. They have shown great potential in homogeneous catalysis. In this field, we report here the crystal structures of [Fe(C_5H_5)($C_{19}H_{24}N_2$)]I, (I), and *trans*- [Fe_2Pd(C_5H_5)2($C_{16}H_{17}N_2$)$_2I_2$], (II). Compound (I) has two iodide anions and two imidazolidinium cations within the asymmetric unit (Z' = 2). The two cations have distinctly different conformations, with the ferrocene groups orientated *exo* and *endo* with respect to the *N*-heterocyclic carbene. Compound (I) can be shown to act as an anion receptor and is used in preparing chiral carbene ligands and their complexes. In complex (II), the ferrocenylmethyl group acts as a pendant group on the N atom of imidazolidin-2-ylidene and shows square-planar coordination around the Pd^{II} metal, which is located on an inversion centre (Z' = 0.5). The ferrocene and benzyl substituents are in a *trans–anti* arrangement.

J.-C. Daran, F. Demirhan, Ö. Yıldırım and B. Çetinkaya

IUCR JOURNALS NEWS

Rapid visualization of hydrogen positions in protein neutron crystallographic structures

Acta Cryst. (2012). D68, 35–41 (http://doi.org/d49jgc)



Although hydrogen atoms are difficult to locate using X-ray crystallography, with neutron crystallography the deuterium isotope can be readily visualized. Neutron analysis, however, has been limited by a number of technical challenges, such as prohibitively long data-collection times. Recent developments in instrumentation and deuterium labeling have dramatically increased the speed of data collection, as illustrated here by the structure of rubredoxin to 1.75 Å resolution, refined against neutron data collected in 14 h and revealing over 70% of deuteron positions without ambiguity.

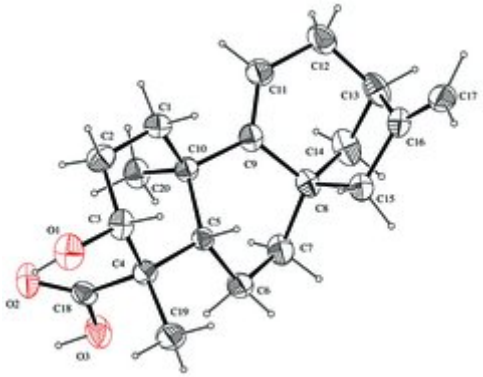
P. Munshi, S.-L. Chung, M. P. Blakeley, K. L. Weiss, D. A. A. Myles and F. Meilleur

IUCR JOURNALS NEWS

(3R,4S,5S,8S,10R,13R)-3-Hydroxykaura-9(11),16-dien-18-oic acid

(3*R*,4*S*,5*S*,8*S*,10*R*,13*R*)-3-Hydroxykaura-9(11),16-dien-18-oic acid

Acta Cryst. **(2012). E68, o526–o527 (http://doi.org/fx56d4)**



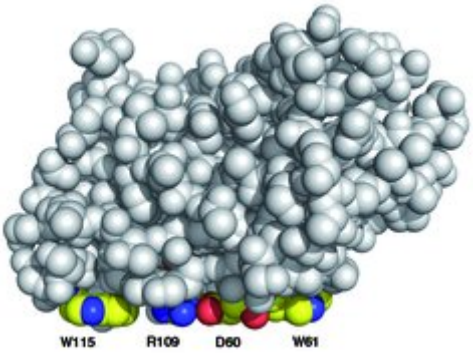
The title compound was isolated during our investigation into the chemical composition and bioactive constituents of *Centipeda cunninghamii* (Asteraceae), an Australian Aboriginal traditional medicine. The *ent*-kaurane possesses a carbon skeleton composed of three six- and one five-membered rings in a chair, twist-boat, half-chair and envelope conformation, respectively. Previous studies have established a relationship between the solution and crystal conformation of this structure class. The absolute stereochemistry of the enantiopure diterpene was established from the optical rotation measurements and comparison to the closely related grandiflorenic acid.

K. D. Beattie, M. M. Bhadbhade, D. C. Craig and D. N. Leach

IUCR JOURNALS NEWS

Structure of CBM3b of the major cellulosomal scaffoldin subunit ScaA from Acetivibrio cellulolyticus

Acta Cryst. (2012). F68, 8–13 (http://doi.org/fx9pds)



Planar face of the CBM3b module from the cellulosome of *Acetivibrio cellulolyticus*. Cellulose-binding residues are indicated.

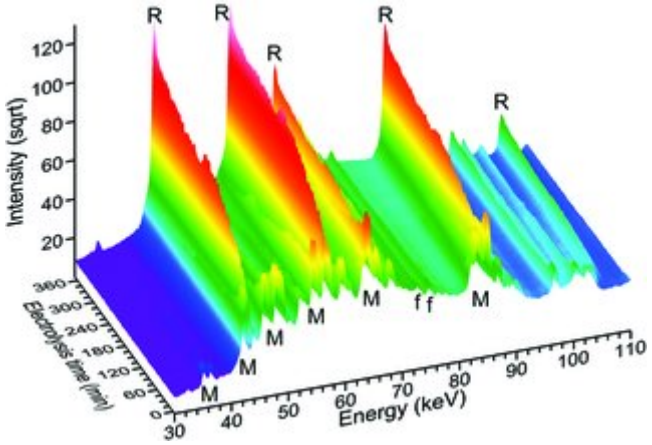
Selected anaerobic bacteria produce a multienzyme cellulosome complex that degrades cellulose. Carbohydrate-binding modules (CBM) target these cellulolytic protein complexes to the cellulose substrate. The binding interaction is driven by a characteristic pattern of aromatic side chains and salt bridges located on a planar surface of the CBM. The structure of the CBM3b from *Acetivibrio cellulolyticus* reveals a particularly compact interacting region consisting of only four amino-acid residues.

O. Yaniv, Y. Halfon, L. J. W. Shimon, E. A. Bayer, R. Lamed and F. Frolow

IUCR JOURNALS NEWS

Quantification of passivation layer growth in inert anodes for molten salt electrochemistry by in situ energy-dispersive diffraction

J. Appl. Cryst. (2012). 45, 28–37 (http://doi.org/dgc7t8)



Accumulated EDXRD patterns of the inert anode as a function of electrolysis time. The main Magnéli (M) phases can be seen transforming into rutile (R).

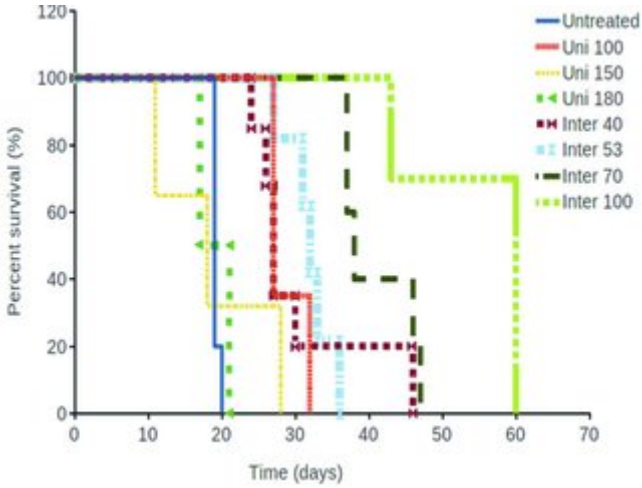
Molten-salt electrochemistry takes place in a hot, aggressive environment. An inert anode operating within such an environment – calcium chloride at 950°C – has been studied using the high penetrating power of energy-dispersive X-ray diffraction (EDXRD). Methodology for performing quantitative crystal-structure-based Rietveld analysis of EDXRD has been developed and applied to this experiment, and has shown the mechanism of change in the phase chemistry of the anode in real time, and under realistic operating conditions. The analysis methodology is generally applicable to any EDXRD data.

M. R. Rowles, M. J. Styles, I. C. Madsen, N. V. Y. Scarlett, K. McGregor, D. P. Riley, G. A. Snook, A. J. Urban, T. Connolley and C. Reinhard

IUCR JOURNALS NEWS

Increase of lifespan for glioma-bearing rats by using minibeam radiation therapy

J. Synchrotron Rad. (2012). 19, 60–65 (http://doi.org/dk88n6)



Survival curves (as a function of time) of 9L gliosarcoma-bearing rats for different doses. The responses of both the control rats (CTRL) and the rats receiving one fraction minibeam radiation therapy in unidirectional and interlaced configurations are shown.

A new radiotherapy technique, minibeam radiation therapy (MBRT), is under development at the European Synchrotron Radiation Facility. It combines submillimetric field sizes (500–700 µm) and a spatial fractionation of dose, which leads to exceptional normal tissue dose tolerances. This might permit the use of potentially curative doses in some radioresistant tumors, like gliomas. This work reports a dose escalation study performed on 9L gliosarcoma-bearing rats. A factor of three gain in mean survival time paves the way for further exploration of different possibilities of MBRT.

Y. Prezado, S. Sarun, S. Gil, P. Deman, A. Bouchet and G. Le Duc

MEETING REPORT

XXII IUCr Congress and General Assembly

Madrid, Spain, August 22-30, 2011

www.iucr2011madrid.es/

The congress brought together nearly 2800 people (1880 standard participants, 360 students, 350 grantees, 65 exhibitors and 113 accompanying persons). 73 countries were represented by 2040 abstracts that were distributed across 98 Microsymposia with 490 oral and 1550 poster presentations. The following reports are grouped by subject matter.



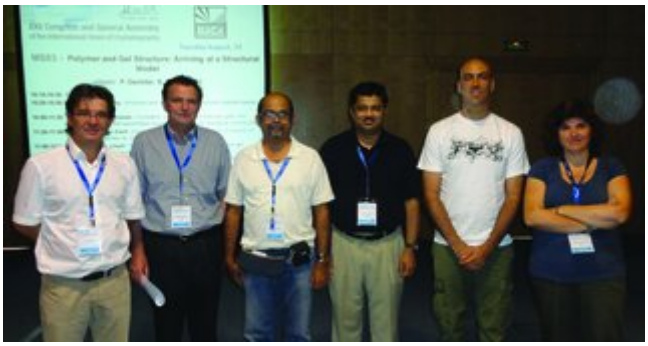




Theory

Polymer and gel structure: arriving at a structural model (MS03)

Chairs: Parthasarathi Dastidar, B. Escuder Gil



Session MS03 Speakers: J. H. van Esch, B. Bagautdinov, P. Dastidar, S. R. Raghavan, G. O. Lloyd and B. Escuder Gil.

This session focused on understanding the (macro)molecular organization found in soft matter - polymers and molecular gels. I. Hamley (U. of Reading, UK) reported on self-assembly studies of peptides related to amyloids, peptide sequences believed to be involved in neurodegenerative diseases such as Alzheimers. S. Raghavan (U. of Maryland, USA) focused on the structural differences between crystalline and amorphous molecular gels and made an analogy with related self-assembling biological systems. J. van Esch (Technical U. of Delft, The Netherlands) reported on controlling soft-matter structure by mixing gelators able to self-assemble orthogonally and on the study of self-assembly in non-equilibrium systems. G. Lloyd (Cambridge U., UK) discussed the relationship between crystallization and gel

formation and the use of molecular gels as media for the crystallization of different polymorphs of drugs. The session ended with B. Bagautdinov (SPring-8, Japan) reporting on structural studies of polyacetylenes.

Crystal structure prediction: practice and applications (MS06)

Chairs: J. Kendrick, S. L. Price

A. Oganov showed how searching for potential structures of simple elements has predicted new high-pressure phases of elements, emphasising the importance of the search algorithm. The microsymposium then shifted to organic molecules, particularly the results of the 2010 blind test of crystal structure prediction, a joint collaborative test of advances in methodology organised by the CCDC. The results of the test were reported by A. Cruz-Cabeza (Málaga U., Spain). Prediction of the structures of some fairly simple small molecules had been successfully demonstrated previously, but this test included more challenging systems: a molecular salt, a large flexible pharmaceutical-like molecule and a novel polymorph of gallic acid monohydrate. At least one correct prediction had been made for each structure, although no method was universally successful. This could be attributed to the problem of accurately evaluating the relative energies. J. van de Streek (Avant-garde Materials Simulation, France) presented post-blind test work on developing and evaluating improved dispersion-corrected density functional periodic quantum mechanical calculations. It has become clear that many organic molecules have a large number of crystal structures that are very close in energy. M. Habgood (University College London, UK) described a method for evaluating structures likely to have static disorder due to configurational entropy outweighing the variation in lattice energy, and presented criteria for assessing this from an examination of the near-symmetry of intermolecular interactions from the low-energy calculated structures. Finally, R. de Gelder (Radboud U., The Netherlands) discussed a method of picking out which crystal structure might approximate that which corresponded to a powder X-ray diffraction diagram. The microsymposium emphasised the advances which have taken place in searching and energy evaluation, and demonstrated applications of the methodology, but still showed the challenges remaining in understanding the kinetics of crystallisation sufficiently to determine which new solid phases might be found.

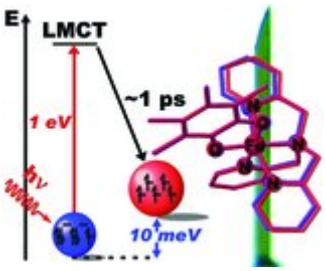
Instrumentation, data collection, processing, analysis, databases

Dynamical structural science (MS45)

Chairs: Pance Naumov, Eric Collet



MS45 Speakers and Chairs: Pance Naumov, Simone Techert, Philip Coppens, R. J. Dwayne Miller, David Fritz, Shunsuke Nozawa and Eric Collet.



Ultrafast structural studies provide atomic level views of dynamical processes in matter, as illustrated here in a photomagnetic material.

Recent advances in pulsed X-ray and electron sources make it possible to track structural reorganization in real time, with a resolution of 100 femtoseconds. Optical pumps coupled to X-ray or electron probe experiments allow the tracking of atomic or molecular motions on their intrinsic time-scale, i.e. the phonon frequency. Dynamical structural science was the subject of a special issue of *Acta Cryst.* (Vol. A**66**, March 2010). In this symposium, state-of-the-art dynamical structural science was presented, dealing with development of X-FEL (D. Fritz, SLAC Nat'l Accelerator Lab., USA) and new electron guns (D. Miller, U. of Hamburg, Germany). New applications of synchrotron pulsed sources to study dynamics of excited states of molecular solids (P. Coppens, SUNY Buffalo, USA), biomolecular systems (S. Techert, GWDG, Germany) and of molecules in solution (S. Nozawa, KEK, Japan) were described.

Data reduction of area-detector measurements (MS68)

Chairs: G. J. Mcintyre, E. Litvinenko



MS68 speakers: Christina Hoffmann, Daniel Chateigner, Arsen Gukasov, Ross Piltz and Loes Kroon-Batenburg.

The focus of talks in the symposia included strategies of data collection with position-sensitive area detectors, methods for correction of distortion and inhomogeneity, subtraction of background, visualization of data containing both Bragg reflections on discrete grids and diffuse scattering, acceleration of and higher accuracy in the extraction of integrated intensities, and application of area detectors to fibre diffraction, texture measurement, and powder diffraction.

D. Chateigner (ENSICAEN, France) gave a lively lecture about the qualitative advances that area detectors have brought to quantitative texture analysis with X-rays and neutrons. Most of the other talks, and the four poster presentations, were devoted to reduction of discrete Bragg data, including Laue diffraction at both reactor and spallation neutron sources, simultaneous measurement of magnetic flipping ratios using area detectors, the latest developments at J-PARC, and methods to get the best from the newest CMOS detectors. Of further note was the talk by R. Piltz (ANSTO, Australia), who described improved methods of reduction of neutron Laue data from the instruments KOALA (ANSTO) and VIVALDI (ILL), which use image-plate detectors, to give significantly better quality in structure refinement.

Automated data processing and structural solution for powder crystallography (MS95)

Chairs: Rosanna Rizzi and Anton Meden

Modern X-ray powder diffractometers have the potential to collect data sets in a matter of minutes. Beamlines are equipped with robots and all aspects of data collection and analysis can be executed in a completely automatic way. B. Toby (Argonne Nat'l Lab., USA) explained how, at the Argonne Advanced Photon Source, they achieve high-throughput remote access by a large number of users *via* automation of all the aspects of the workflow (*i.e.* requests for sample-mounting kits, programming of the data-collection parameters, post-collection data reduction, and sample storage). This uniform sample management is linked to computer programs for data analysis that carry out, automatically and quickly, the complete structure determination process. A. Altomare (CNR, Italy) discussed new algorithms introduced in the *EXPO* program for automatic and efficient *ab initio* crystal structure determination. L. McCusker (ETH Zurich, Switzerland) illustrated the application of a charge-flipping algorithm to determine complex zeolite structures. The combination of the algorithm with HRTEM and PED techniques

was also explained. R. Oishi-Tomiyasu (Inst. of Materials Structure Science, Japan) discussed the main functions of the *Conograph* program for primitive unit-cell determination, lattice symmetry determination and parameter refinement. M. Milanesio (U. del Piemonte Orientale, Italy) showed how structural information on a subset of atoms can be selectively obtained when the sample is subject to a periodically varying external stimulus (temperature, pressure, concentration *etc.*).

Chirality in the solid state, from organic molecules to chiral MOF and helical materials (MS87)

Chairs: Susan Bourne and Berta Gomez Lor



Session MS87 Speakers and Chairs: Mikiji Miyata, Iwona Justyniak, Nikoletta Báthori, Susan Bourne, Berta Gomez-Lor, Giancarlo Terraneo and Simon Parsons.
The significant role played by chirality in chemistry and biology was highlighted in talks that ran the gamut from inorganic coordination complexes to large and small supramolecular systems, utilizing a range of bonding and intermolecular intractions.

M. Miyata (U. of Osaka, Japan) began the session with a somewhat provocative suggestion that it is possible to assign handedness to all helices. After demonstrating the assignment of handedness to two-fold helices by invoking a tilt-chirality, he illustrated his talk with examples of chinchona alkaloid structures that commonly crystallize in either $P2_1$ or $P2_12_12_1$. After assigning the helices as either right- or left-handed, he suggested a modification be made to their space group representations. The suggestion generated animated discussion from the floor.

I. Justyniak (Polish Acad. of Sciences, Poland) used the chinchona alkaloids, specifically chinchonine and chinchonidine, as ditopic ligands in coordination polymers. Using these ligands to connect Aluminium ions gave rise to homochiral helical channel compounds, with either coordination or supramolecular interactions holding the helices in place. The channels have a chiral nature and can be used to effect enantiomeric separation of liquid guests. They are also able to absorb a range of gases under relatively mild conditions.

N. Báthori (Cape Peninsula U. of Tech., South Africa) uses organic host compounds with imperfect selectivity for guests to probe the mechanism by which chiral discrimination can be effected through crystallization. Combining NMR or HPLC measurements with crystal structure analysis in compounds with mixed guests, she elucidated principles guiding the inclusion of one enantiomer over another. Hirshfeld surface analysis applied to the supramolecular units proved particularly valuable in probing the intermolecular interactions at play in related enantiomeric structures and allowed her to draw some conclusions about the driving forces in the separation crystallization of these compounds.

G. Terraneo (Politecnico de Milano, Italy) has used halogen bonding as an intermolecular interaction to produce chiral compounds from achiral moieties. After providing an overview of halogen bonding, a hot topic in crystal engineering, he presented results for a range of cocrystals produced with long-chain diiodoperfluorocarbons (PFCs). The CSD contains only 45 structures of PFCs with 8 or more carbons, while the cocrystals reported in this talk utilise $I(CF_2)_{12}I$ as coformer, taking these crystals to the crystalline/liquid interface. Through these examples Terraneo illustrated how the halogen bond can be used to overcome the low affinity of PFCs and hydrocarbons and, furthermore, how long-chain PFCs without chiral centers can be induced to crystallize in chiral space groups. S. Parsons (U. of Edinburgh,

UK) presented some new approaches to refining the Flack parameter which gives a measure of the correct assignment of absolute configuration.

Automation of data collection and remote control of experiments (MS13)

Chairs: Olof Svensson, Masaki Yamamoto

This microsymposium focused on how automation and remote access can enhance user-friendliness and efficient use of often limited beamtime available at synchrotrons. After an introduction by M. Yamamoto, A. Popov presented the current status of the *BEST* program. The presentations given by A. Gonzales (SSRL, USA), K. Hasegawa (Spring8, Japan) and S. Wasserman (APS, USA) described their use of *BEST* and gave an overview of the state-of-the-art of automation and remote data collection on MX beamlines at three major synchrotron radiation sites. In the last talk of the session R. Cooper presented the theory and implementation of improving experimental results by selectively re-measuring the most relevant reflections for the particular study.

Developments and directions for crystallographic databases (MS27)

Chairs: S. Gražulis, J. Westbrook

Crystallographic data resources face a variety of challenges. The availability of high-bandwidth internet connectivity offers new possibilities for data access and sharing; at the same time crystallographers expect deeper annotation and more robust data quality indicators from modern internet-based resources. These challenges were discussed by the three invited speakers representing the Crystallography Open Database (COD), the Cambridge Crystallographic Data Center (CCDC) and the Worldwide Protein Data Bank (wwPDB).

Maintaining high-quality data resources inevitably requires careful and detailed data curation to ensure database consistency, homogeneity and reliability. All of the speakers in this session reported how their resources address the technical, social and resource requirements associated with this data curation. The participants were also sensitive to the need to provide data consistency while faithfully preserving the author-provided primary data content. While the infrastructure for data curation has been well established in the PDB and CCDC archival resources, this is a area of active development for initiatives such as COD.

The availability of high-quality structural data also makes possible new approaches for data analysis, mining and prediction. New graphical query interfaces for inorganic data require advanced mathematical concepts to retrieve different types of structures efficiently, and application of fractal geometry may be necessary to analyze trends hidden in raw data files.

Other techniques

Electron diffraction and crystallography (MS79)

Chairs: P. N. H. Nakashima, C. T. Koch



Session MS79 speakers and chairs: Philip Nakashima, Christoph Koch, Andrew Stewart, Ray Withers, Peter Oleynikov, Andrew Johnson and Kenji Tsuda

The talks and posters in this session covered electron diffraction and imaging techniques for the solution of crystal structures (including structures with unit-cell volumes as large as 38.3 nm^3) and

characterization of nanomaterials. A prominent theme was the extension of electron diffraction beyond 2D patterns to explore the 3rd dimension. This was presented in several different flavors, including classical convergent-beam electron diffraction (CBED), precession electron diffraction (PED), automated diffraction tomography (ADT) and the very recently established large-angle rocking-beam electron diffraction (LARBED) and rotation methods.

Biological neutron scattering and deuteration (MS82)

Chairs: Trevor Forsyth, Joanna Krueger

This microsymposium focused on the advantages of using neutron scattering in combination with sophisticated deuteration approaches to enhance structural studies of macromolecular systems in crystals, solutions and partially ordered systems. The presentations included studies that have provided new information on the location of protons and structured water in proteins (information of central importance in optimising ligand interactions), solution scattering studies where contrast variation has been used to characterize different regions of a macromolecule in relation to function, and reflection work relevant to biological interfaces. A. Podjarny (IGBMC, France) described his crystal structure determination at 293 K of a perdeuterated type-III antifreeze protein (AFP). The water structure was clearly visible from the neutron diffraction study, demonstrating an interesting tetrahedral geometry that explains the specificity of these AFPs for the ice *versus* liquid structure of water. O. Byron (U. of Glasgow, UK) described a neutron scattering contrast-variation study of the pyruvate dehydrogenase (PDH) complex. Solution techniques have been used to model specific parts of the complex and SANS has been used to study the stoichiometry of subunit associations by titrating a specifically deuterated subunit (E2) with a second subunit E3BP. These results, used in combination with other biophysical techniques, resolved a conflict between current models of the PDC core and allowed clearer visualization of the subunit content and organization. M. Cuypers (Keele U., UK) discussed the difficulty of reliable X-ray data acquisition from the reduced (Fe^{2+}) form of the perdeuterated rubredoxin given the effects of beam-induced oxidative degradation. This problem was resolved in a high-resolution neutron crystallographic analysis of both Fe^{2+} and Fe^{3+} forms of the protein. The study correlated redox properties with associated protonation shifts and detected H_3O^+ ions in the structure. L. Coates (ORNL, USA) described the protonation states and H-bonding network in the ground state active site of β-lactamase. T. Darwish (ANSTO, Australia) described collaborating with structural chemists to design deuterated compounds that increase the scope of neutron diffraction, scattering and reflectometry experiments.

Industrial applications of SAXS and SANS (MS04)

Chairs: Robert Knott, Aldo Craievich

M. Shibayama (Tokyo U., Japan) presented examples of the use of contrast-variation SANS. He demonstrated that catalyst inks consist of dendritic clusters of carbon nanoparticles surrounded by ionomers, with platinum located in the ionomer layers. This structure makes platinum more accessible and therefore more efficient.

J. Doucet (Novitom, France) described the use of micro-focused SAXS to determine the asymmetric distribution of proteins in hair fibers. Among other things, such information is valuable in developing products that make curly hair straight and straight hair curly. D. Londono (DuPont, USA) presented SAXS studies of the interaction between silica particles and polymers. A key finding was that, during nanocomposite formation, high molecular weight polymers freeze a monodispered population of silica particles to produce a well-dispersed material.

A strategy for developing novel materials-by-design was outlined by A. Allen (NIST, USA). He described how the contrast-variation SANS technique is used to determine the composition and density of calcium silicate hydrates in cured cement. H. Brand (CSIRO/ANSTO, Australia) presented a study of a series of jarosite compounds that form crystalline structures having an impact in mineral and environmental industries.

The posters included information on instrumentation development, structural investigations of polymers under shear, and thin films and lignins related to fuel production from biomass.

Macromolecules

Hybrid methods: the EM-crystallography interface (MS02)

Chairs: Eva Nogales, Jorge Navaza

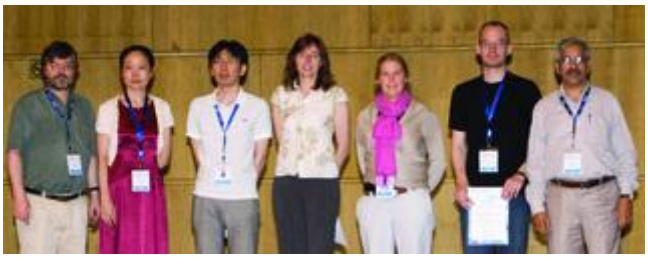


Session MS02 speakers and chairs: Phillip Heuser, Ines Muñoz, Roland Beckmann, Eva Nogales, Jack Johnson, Hong Zhou and Jorge Navaza.

The structural characterization of large macromolecular assemblies often requires the use of multiple and complementary techniques in order to obtain the maximum mechanistic insight. Cryo-EM structures in the subnanometer regime, combined with crystallographic atomic models of components, can be a very powerful combination to mechanistically define essential biological processes. J. Johnson (Scripps Research Inst., USA) utilized X-ray crystallographic data, time-resolved SAXS data and cryo-EM viral structures obtained from coexisting populations of viruses to map the structural pathway or reorganization in the viral capsid during the pH-controlled maturation of the virus. While SAXS provided a read out in real time of the overall changes in the capsid volume, the cryo-EM studies described the viral populations that coexist under a finite number of defined conditions at subnanometer resolution. The latter could then be interpreted with pseudo-atomic detail using crystallographic information and molecular dynamics.

Cell signalling and protein-protein interactions (MS22)

Chairs: Michael Parker, Madhusoodan Hosur

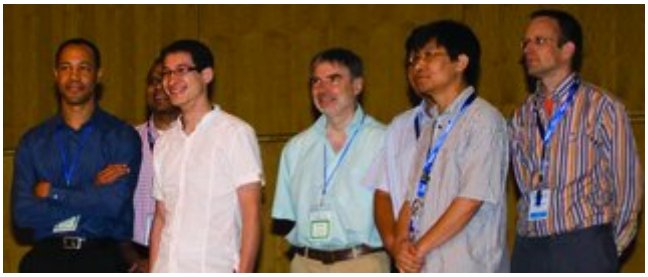


Session MS22 speakers and chairs: Michael Parker, Jia-Wei Wu, Yoshinori Hirano, Christine Gee, Sarah Teichmann, Christian Anderson and Madhusoodan Hosur.

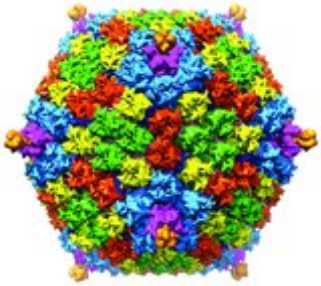
This microsymposium focused on the role of PPI's in cell signalling. The talk given by S. Teichmann (MRC Lab, Cambridge, UK) described analysis of PPI's using bioinformatics tools. Her analysis revealed: 1) evolutionary constraints on surface residues forming sticky patches, and 2) the predictability of binding-induced conformational changes through relative accessible surface area calculations. The next two talks focused on the largest family of signal transducers in the cell: protein kinases. J.-W. Wu (Tsinghua U., China) presented her work on AMP kinase, highlighting the importance of obtaining structures that are as complete as possible. Discovery of activators of AMPK could lead to a 'fat' pill! C. Gee (U. of California, Berkeley, USA) described the structure and function of a pseudokinase. The final talks provided fascinating insights into molecular recognition: how the 'small' molecule vitamin B_{12} is taken up by cells (C. Anderson, Aarhus U., Denmark) and how 'larger' molecules are recognized by an atypical myosin (Y. Hirano, Nara Inst., Japan).

Viruses and viral proteins (MS29)

Chairs: Fasseli Coulibaly, Ying-Fang Liu



Session MS29 speakers and chairs: (front) Fasseli Coulibaly, Vijay Reddy, Marc Kvansakul, Felix Rey, Luis Castillo; (back) Ying-Fang Liu, Mark van Raaij.



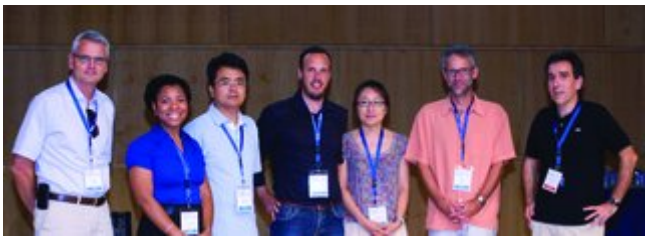
The microsymposium 'Viruses and Viral Proteins' featured presentations by M. J. van Raaij, M. Kvansakul and L. Castillo that represented the multiple aspects of structural virology with emphasis on understanding the assembly, evolution and virulence of viruses.

In addition, the structure of human adenovirus presented by Vijay Reddy stood out as an impressive feat allowing visualization of the intricate network of major and minor structural proteins in the virion. The cryoEM structure of adenovirus determined independently (MS02, Hong Zhou) provided a rare opportunity for meaningful comparison of data obtained by X-ray crystallography and cryoEM. A clear point of divergence was the assignment of a four-helix bundle on the capsid exterior to protein IIIa or protein IX, depending on the study.

Finally, Felix Rey introduced the structure of an EFF-1 homotypic fusion protein essential to organogenesis in *C. elegans*. The presentation ventured outside the virus world...only to show that these cellular proteins are homologous to viral class II fusion proteins. This groundbreaking discovery opens exciting avenues to understanding the function of fusion machineries from a totally new perspective. The ensuing discussion initiated by Jack Johnson and Michael Rossmann examined frameworks that could account for this unanticipated evolutionary link.

Understanding bacterial pathogenesis (MS36)

Chairs: Armando Albert and Dirk Heinz



Session MS36 speakers and chairs. Dirk Heinz, Breann Brown, Xinquan Wang, Jérôme Le Nours, Hae Joo Kang, Thilo Stehle and Armando Albert.

This microsymposium highlighted the structural basis for infection and immunity. X. Wang (Tsinghua U., China) reported on the structure of the cytokine interleukin-1β (IL-1β) and its interactions with the IL-1 receptor type I (IL-1RI) and IL-1 receptor accessory protein (IL-1RAcP). Using X-ray crystallography, site-

directed mutagenesis and surface plasmon resonance (SPR), he was able to decipher the mode of assembly of this cytokine-receptor complex. T. Stehle (U. of Tuebingen, Germany) discussed the high-resolution structure of a staphylococcal autolysin which provided detailed insights into the enzymatic function of this peptidoglycan hydrolase. Small-angle X-ray scattering (SAXS) experiments were used to analyze molecular flexibility and to provide a model for bacterial cell wall recognition.

H. J. Kang (U. of Auckland, New Zealand) presented new results on the structure, assembly and function of pilins from pathogenic gram-positive bacteria. Pilins polymerize on the bacterial surface to from pili, which are essential for bacterial conjugation and inter-species DNA exchange. Using structural biology and mass spectrometry he could identify unusual isopeptide bonds further cross-linking pilins. J. Le Nours (Monash U., Australia) reported the crystal structures of a Shiga toxigenic *E. coli* AB5 bacterial toxin and individual subunits that are important virulence factors for several major bacterial pathogens. B. Brown (Brown U., USA) described so-called toxin-antitoxin (TA) complexes that are heavily upregulated in persister cells belonging to bacterial biofilms that are notoriously resistent towards antibiotic treatment. Extensive structural and functional analysis on the MqsA/R TA system showed that it acts as a master regulator of *E. coli* biofilm formation, thus representing a new target for antibiotic therapy.

Complementary biophysical methods: adding value to protein structures (MS51)

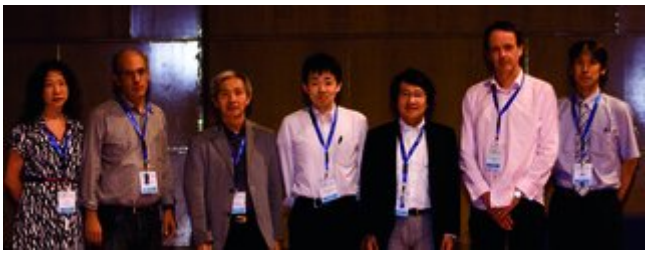
Chairs: Nathan Cowieson, Dorothy Beckett



Session MS51 speakers and chairs: Remy Loris, Nathan Cowieson, Diana Tomchick, Dorothy Beckett, Ed Egelman, Nicole LaRonde LeBlanc, Jaqueline Cherfils.
This session highlighted the power of combining X-ray crystallography with other techniques in elucidating structure-function relationships in biomolecular systems. A recurring theme in the presentations was the integral role that plasticity plays in proteins. R. Loris's (VIB-VUB, Belgium) talk on the toxin:antitoxin system illustrated how application of NMR spectroscopy, SAXS, equilibrium binding measurements and X-ray crystallography enabled determination of the roles of disorder-to-order and protein association in this system. E. Egelman (U. of Virginia, USA) combined high-resolution cryoEM with X-ray crystallography to uncover the range of helical filamentous structures accessible to nearly identical monomeric subunits of actin, flagellin and pilin. J. Cherfils (CNRS, France) presented results of NMR spectroscopy, SAXS and X-ray crystallography in demonstrating the roles of transient unfolding and enhanced dynamic states in dictating alternate specificities of the structurally identical small G-proteins. D. Tomchick (U. Texas Southwestern, USA) discussed the contributions of SAXS, X-ray crystallographic and NMR analysis to determining the roles of structure and internal dynamics in multi-level regulation of the vav1 signaling protein. N. LaRonde LeBlanc (U. of Maryland, USA) demonstrated that the combination of analytical ultracentrifugation, kinetic analysis of enzyme function and X-ray crystallography yields information to enable formulation of a model for control of enzyme function *via* regulated oligomerization.

Hot structures in biology (MS64)

Chairs: Tsuyoshi Inoue, Se Won Suh



Session MS64 speakers and chairs: Hao Wu, Alekos Athanasiadis, Se Won Suh, Hiryoyoshi Matsumura, Shigeyuki Yokoyama, Michael Lawrence and Tsuyoshi Inoue.
A. Athanasiadis (Gulbenkian Inst. of Science, Portugal) presented the unstable structure of the Z-to-Z junction found in Z-DNA, which was stabilized by Za, the Z-DNA binding domain of the RNA editing enzyme ADAR1. He showed the difference in the stacking interactions between B-to-Z and Z-to-Z junctions. Shigeyuki Yokoyama (U. of Shizuoka, Japan) described the distinctly different structures of two type II aminoacyl-tRNA synthetases of (alanyl- and histidyl-tRNA synthetase) in complex with their cognate tRNAs, respectively, and showed the mechanisms of tRNA recognition. The indirect mechanism of aminoacyl-tRNA synthesis was also described on the basis of complex structures with tRNAs. Both speakers offered insights into the structures of DNA and the translation machinery.

Other speakers described structures involved in cellular signaling. H. Matsumura (Osaka U., Japan) presented the binary complex structure of an intrinsically disordered protein, CP12, and glyceraldehyde-3-phosphate dehydrogenese (GAPDH), the structure of phosphoribulokinase (PRK), and the proposed ternary complex structure of CP12/GAPDH/PRK, regulating the Calvin cycle in plants. M. Lawrence (Walter and Eliza Hall Inst., Australia) described the structure of insulin in complex with Site 1 on the insulin receptor (IR). Site 1 consists of elements of the first leucine-rich repeat domain (L1) of one receptor monomer and the C-terminal segment (αCT) of the α-chain of the second monomer. The αCT helix was repositioned upon binding of the insulin B-chain, following the binding toward Site 2 within an intact IR dimer. H. Wu (Weill Cornnel Medical College, USA) presented the structure of the Myddosome death domain complex in the Toll-like receptor and IL-1 receptor superfamily pathway and also the inhibitor-bound structure of IKKβ which is activated by IRAK in the subsequent gene transcription. She showed the high-order oligomerization in TLR/IL-1R signaling. Structural information on proteins bound with DNA and RNA and complex structures in signal transduction can provide deeper insights into functional mechanisms of systems biology.

Transcription and translation (MS78)

Chair: Anders Liljas



Patrick Cramer



Marat Yusupov



Anders Liljas, Chair

P. Cramer (Gene Center of the U. of Munich, Germany) described eukaryotic gene transcription and three different RNA polymerases that have many common proteins as well as unique ones. The complex goes through a number of conformational changes during the functional cycle, including movement of the RNA and DNA components through tilted and regular conformations while maintaining base-pairing and the binding of a number of factors to a very long C-terminal tail domain that depends upon on site specific phosphorylation.

M. Yusupov (IGBMC, France) described purification of homogenous yeast ribosomes after glucose starvation that produces crystals that diffract to 2.6 Å resolution. More than 5000 nucleotides are placed in the current 3.0 Å map as well as 78 of 80 proteins. The expanded segments of rRNA and the additional proteins compared to bacterial ribosomes are all on the external sides. The asymmetric unit contains two 80S ribosomes in different stages of ratcheting. Here it was observed that the bases of the small subunit that stabilize the cognate interaction between mRNA and tRNA were in very different locations. The most remarkable situation was the binding of the stress response factor Stm1 to part of the binding site for the mRNA.

T. Lavy (Cold Spring Harbor Labs, USA) described the three primary proteins of the GAL regulon in *S. cerevisiae*, Gal3p (transducer), Gal4p (transcriptional activator) and Gal80p (repressor). Through crystal structures of different complexes much of their interplay could be described in detail. Through mutants, primarily of Gal80p, dramatic conformational and functional effects could be studied.

K. Kihira (Osaka U., Japan) described novel studies of the bacterial release factor 3 (RF-3). Two different forms of the protein could be isolated late in the growth phase, one containing GDP and the other ppGpp. This could be identified first from electron density and subsequently biochemically. The ppGpp is part of the stringent response and probably due to the large extent of uncharged tRNA at the late stage in bacterial growth.

Periodicity

Methods and software for perodic and aperiodic crystals (MS69)

Chairs: Michal Dusek, Iian-Mao Peng

The symposium began with talks on the state of the art of electron microscopy, image simulation and surface structure determination using electron based techniques. In 'Modeling thermal scattering and solving structures using *Z*-contrast imaging', L. J. Allen (U. of Melbourne, Australia) emphasized the utilization of the thermal diffusely scattered electrons in atomic resolution imaging *via Z*-contrast mechanism, and the EDX mapping down to a single atom column. In '$SrTiO_3$ surface structure from diffraction and DFT: homologous series and glasses', L. D. Marks (Northwestern U., USA) emphasized the difficulties of conventional crystallographic methods for the determination of complex oxide surface structures. O. Gourdon (Juelich Center for Neutron Science, USA) described how to use ToF data provided by the Powgen instrument in Oak Ridge to calculate magnetic structures. J. J. Lovelace (Eppley Inst., USA) talked about simulations of modulated protein structures. S. Deloudi (ETH Zurich, Switzerland) discussed periodic average structures associated with *n*-fold quasiperiodic tilings (n = 7-15).

What is order and how can we measure it? (What kinds of matter diffract?) (MS84)

Chairs: Marjorie Senechal and Uwe Grimm

The diffraction pattern of Penrose tilings (first shown at the 1981 Ottawa IUCr congress) and the discovery of quasicrystals a year later raised a fundamental question: if lattices and Bragg peaks are not synonymous, then what is a crystal? Between 120 and 150 people attended our Microsymposium to discuss the current state of this question. Our two titles - 'What is order and how can we measure it?' and 'What kinds of matter diffract?' reflect thirty years of multi-disciplinary research and debates. As our first speaker, W. Steurer (ETH Zurich, Switzerland), explained, we now understand that order/disorder are not opposites: instead, they encompass a spectrum. The spectrum can be measured by 'complexity', but different complexity measures - such as algorithmic, symbolic, structural and diffraction pattern - do not always agree. Nor do researchers agree on which has priority. R. Mosseri (U. Pierre et Marie Curie, France) and V. Kolosov (Ural State U., Russia) discussed another aspect of disorder - geometric frustration - and its representations in curved spaces, and Shelomo Ben-Abraham (Ben-Gurion U., Israel) returned to the complexity theme. We held an open discussion of the issues raised by the speakers. The debate was intense and illuminating. The Commission on Aperiodic Crystals still has work to do!

Crystal chemistry and physics of modulated crystals (MS88)

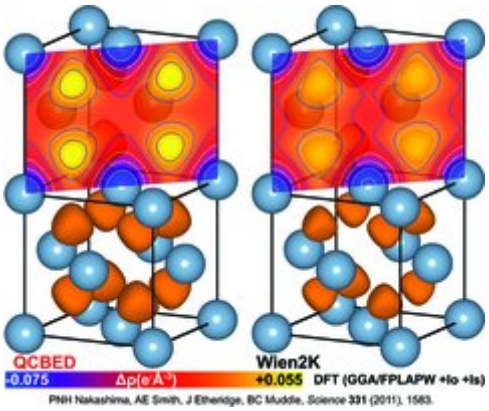
Chairs: J. Haderman, A. Schönleber

Modulated and composite crystals are being characterized in inorganic materials, minerals and molecular compounds. K. Friese (U. of Basque Country, Spain) and C. Basilio Pinheiro (U. Federal de Minas Gerais, Brazil) presented overviews of incommensurate modulations occurring in minerals and molecular compounds, respectively, with examples from their work. A. Abakumov (U. of Antwerp, Belgium) described a completely homologous series of incommensurately modulated perovskite structures, tunable in cation as well as anion content. O. Perez (CRISMAT, France) discussed the likelihood that many of the crystals now described as disordered could actually be modulated crystals. N. Van Tri (Hanoi U. of Science and Tech., Vietnam) tried to put aperiodic structures into relation to nanostructures.

Bonding

Chemical bonds in aluminium (MS41)

Chairs: N. Bouhmaida, C. Jelsch

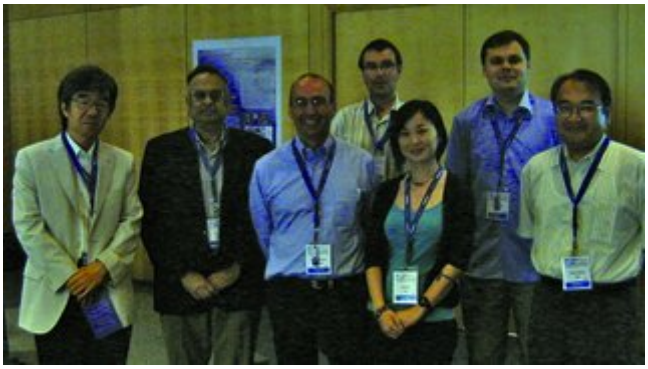


P. N. H. Nakashima (Monash U., Australia) described the use of quantitative convergent-beam electron diffraction (QCBED) to determine the bonding electron density in aluminium. The results resolved a long-standing disagreement based on several theoretical and experimental investigations as to whether bonding in aluminium is octahedrally or tetrahedrally coordinated.

A density functional theory (DFT) first-principles calculation of the ground-state electron distribution was also performed. The QCBED and DFT determinations show that the bonding electron density is concentrated exclusively in the tetrahedral interstices. The results were correlated with the mechanical anisotropy of aluminium and the morphologies of precipitates that form in aluminium alloys.

Electron momentum and spin densities in correlated electron systems (MS48)

Chairs: Bernardo Barbiellini, Masa-Hisa Ito

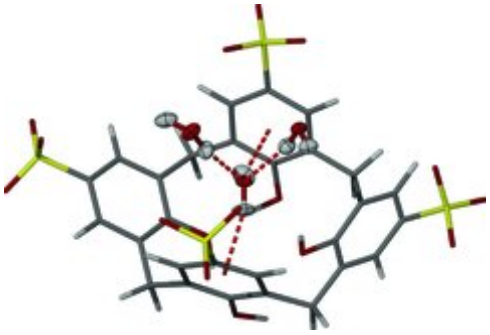


Session MS48 speakers and chairs: (front) Masa-Hisa Ito, Arun Bansil, Bernardo Barbiellini, Maki Okube, Yoshiharu Sakurai; (back) Stephen Dugdale, Alexey Baranov.

Magnetism and superconductivity are two pillars of the physics of correlated electron systems. The techniques presented in this session for probing the spin polarisation in spintronic materials can have an important industrial impact, while the momentum-density studies on the effect of hole doping in high-temperature superconductors can give an indication of the correctness or applicability of many competing models of high-temperature superconductors. S. Dugdale (Bristol U., UK) presented results of recent Compton scattering measurements performed on optimally Co-doped $BaFe_2As_2$ pnictide superconductor. These data show that the Fermi surface of this compound has a nontrivial 3-dimensional shape, which can only be explained by *ab initio* calculations, where the As atomic position can relax. M. Okube (Tokyo Inst. of Technology, Japan) used resonant X-ray magnetic scattering to determine the electronic character of the Verwey transition and help resolve a long-standing debate regarding the nature of this transition. A. Bansil (Northeastern U., USA) used high-resolution Compton scattering to image holes in cuprate high-temperature superconductors and aid in understanding the metal-insulator transition (MIT) in complex materials. A. Baranov (Max-Planck-Inst., Germany) described how insight into the MIT can also be obtained by analyzing electronic motion in real space. He introduced electron localization indices showing the degree of electron-pair exchange inside and between various regions of space. Y. Sakurai (SPring8, Japan) presented a method based on magnetic Compton scattering which provides unique information on the transport and magnetic properties of half-metallic materials. The technique has been applied successfully to ferromagnetic manganites.

Hydrogen bonding: from the solid state to solutions (MS90)

Chairs: Alan Soper, Mark Tuckerman



p-Sulfonatocalix[4]arene with hydrogen-bonded water molecules.

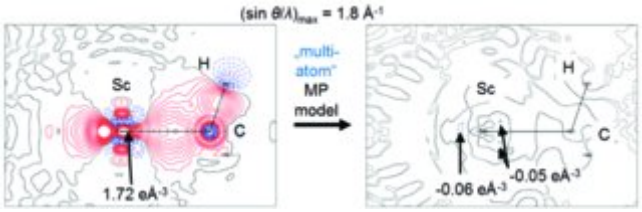
A. Michaelides (U. College London, UK) gave an introduction to the combined technique of path-integral molecular dynamics with density functional theory. He explored the transition of double-well hydrogen-bond potential that occurs in Ices VIII and VII, with two possible locations of the hydrogen atom, to the single-well potential of Ice X, where the hydrogen has only one site with significant broadening along the O-O axis. C. Bull (U. of Edinburgh, UK) described experimental studies of hydrogen bonding under

pressure using diamond anvil and Paris-Edinburgh pressure cells and neutron scattering. C. Jelsch (CNRS, France) described multi-polar atom electron-density calculations of hydrogen bonds, revealing the weak lone pairs in water, hydroxyl and carbonyl groups, which disappear in the oxygen ester group. K. Fucke (Durham U., UK) described the small water clusters encapsulated in p-sulfonatocalix[4]arene. These molecules contain four phenol-like rings with the -OH groups pointing into the centre where they form hydrogen bonds with water. Such molecules are studied as models for drug delivery.

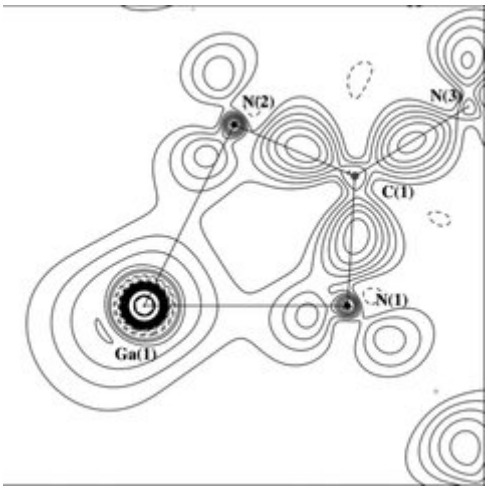
Descriptors of electronic structure and chemical bonding (MS34)

Chairs: Louis J. Farrugia, Angel Pendás

The first two talks in the session had a marked methodological character, showing state-of-the-art descriptors in chemical bonding from real-space analyses. E. Matito (Basque Country U., Spain) provided a detailed account of multicenter bonding as related to aromaticity measures. It has become clear that very good correlations with a large set of aromaticity indices proposed in the literature have been found with the so-called multicenter delocalization descriptors, which involve the *n*-central moments of the electron population in different real-space basins. Unfortunately, the calculation of these quantities is far from trivial, requiring *n*th-order reduced density matrices in the *n*-center case. Matito clearly illustrated these shortcomings, and showed how simplified versions of the indices in terms of the first-order density may be obtained, thus approximating the *n*th-order matrices in different ways. P. Bultinck (Ghent U., Belgium) introduced the iterative Hirshfeld procedure to the crystallographic community. This is a partitioning method based on the Stockholder prescription that overcomes the severe dependence of traditional Hirshfeld atoms on the chosen atomic reference densities. He clearly showed how this partitioning may be used as an extremely cheap alternative to other widely used Atoms in Molecules, like those coming from the Quantum Theory of Atoms in Molecules of Bader and coworkers. The iterative Hirshfeld atoms were shown to be independent of the starting reference, and very transferable among different systems in similar chemical environments. Bultinck also emphasized the quality of their charged multipolar moments, which make the Hirshfeld-I atoms a good alternative for several crystallographic problems.



The remaining three talks dealt with applications to experimental (and potentially experimental) systems. The talk by G. Eickerling (U. of Augsburg, Germany) emphasised two important points in the accurate modeling of electron densities for heavier elements, (*a*) the importance of including relativistic corrections in providing accurate densities and (*b*) the necessity of including core polarizations in multipole modeling of high-resolution theoretical static structure factors. The model systems studied included $M(CH_3)$ (M = Sc, Y, La) and they were successfully dealt with by a simple extension of the Hansen-Coppens pseudo-atom multipole model using two or more pseudo atoms per heavy-atom site. As expected, these core polarisation effects become increasingly important as the resolution of the data increases.



A very similar approach was reported by J. Overgaard (Aarhus U., Denmark) in the combined experimental and theoretical study on an *N*-heterocyclic carbene complex of Ga(I). A standard Hansen-Coppens pseudo-atom modeling of the experimental and theoretical data gave quite unsatisfactory residuals, which were resolved by treatment of the core density as two separate pseudo atoms. This implicit rescaling gave excellent agreement between theory and experiment for the Laplacian properties, which showed intriguing evidence for the presence of a lone pair on the Ga(I) site. The metal-ligand charge distribution was consistent with a good σ-donor ligand with poor π-acceptor properties.

The final talk by S. Mondial (U. of Bayreuth, Germany) dealt with an experimental charge-density study on γ-B_{28}, a fascinating new allotrope of boron reported in recent independent studies by Organov *et al.* and Zarechnaya *et al.* This consists of icosahedral B_{12} units which are linked directly by B-B interactions and also through isolated B_2 units. From the topological properties of ρ(**r**) and $\nabla^2\rho(\mathbf{r})$, it was concluded that there is a 2c-2e bond between the B atoms of the B_2 units and these are linked to the icosahedra by 3c-2e bonds. A Bader partioning gave rise to small charges on the B atomic basins in this formally covalent material.

To be continued in the next issue.

It's not too late to report on your session. We are still accepting reports for inclusion in future issues.

AWARDS AND PRIZES

The 2011 Gregori Aminoff Prize in Crystallography goes to Addadi and Weiner

This Prize rewards contributions in crystallography, including areas concerned with the dynamics of the formation and determination of crystal structures. The Royal Swedish Academy of Sciences awarded the 2011 Prize to Lia Addadi and Stephen Weiner. Addadi is a Dorothy and Patrick E. Gorman Professor and Chair of Biological Ultrastructure at the Weizmann Inst. where she studies the interactions between crystals and proteins, antibodies, or whole cells. Weiner is the Walter and Trude Borchardt Professorial Chair in Structural Biology at the Weizmann. His research focuses on biomineralization and archaeology. Addado and Weiner have successively identified the biologically controlled texture of biominerals that occurs along specific crystallographic planes on protein crystals, which controls their formation, orientation, size, shape and assembly, and gives rise to the complex shapes of many beautiful marine organisms.

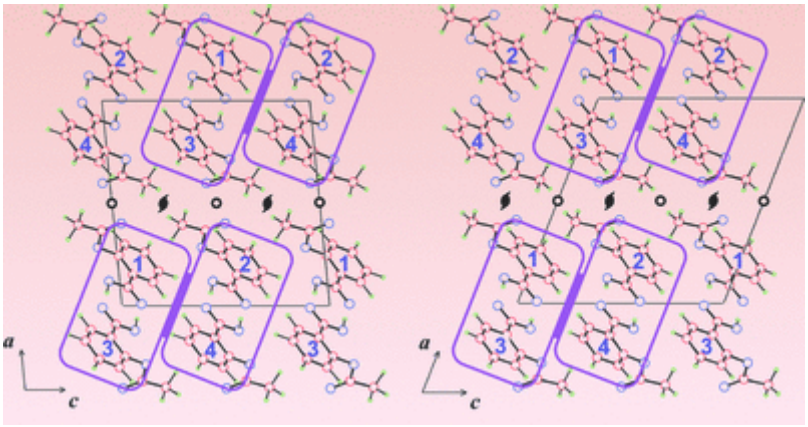
AWARDS AND PRIZES

Brunger wins inaugural DeLano Award

The American Society for Biochemistry and Molecular Biology (ASBMB) has created the DeLano Award for Computational Biosciences in memory of Warren DeLano, the developer of the molecular graphics program *PyMOL*. The inaugural award will be presented to Axel T. Brunger (Stanford U.) who developed *X-PLOR*. His program enabled scientists to refine three-dimensional crystal structures, which previously took months, in just days.

NOTICE

Acta C publishes virtual issues on polymorphism and absolute structure



Following up on the success of its virtual issue on polymorphism (http://journals.iucr.org/special_issues/2011/polymorphism/), *Acta Crystallographica Section C* is planning to publish its second virtual issue towards the end of 2012. This next issue will include papers in which an absolute structure determination (successful or unsuccessful) is reported.

The concept of virtual issues of *Section C* is a new initiative designed to make it easier for readers to find papers relevant to their field of interest, thus increasing the visibility and impact of those papers, and consequently the attractiveness of the journal to authors. Online publishing readily facilitates the creation of virtual issues, which can be used to bring together and highlight papers on specific topics that have recently been published in the journal. The contents page of the virtual issue then provides suitable links to the original papers.

The unambiguous determination of absolute structure, particularly where the absolute configuration of an enantiomerically pure chiral molecule is needed, is important not only for synthetic and natural product chemists, who wish to fully characterize their products, but can be a critical step for the pharmaceutical industry, where opposite enantiomers of a drug can have quite different biological properties.

One of the remaining difficulties since the introduction of the 'Flack parameter' [Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881] has been a reliable absolute structure determination for materials containing only light atoms (e.g. C, H, N, O) when no other chemical or physical knowledge about the chirality of a substance is available. However, there have been recent advances in methods for evaluating the contribution of resonant scattering to reflection intensities (the Friedel differences), while the advent of dual radiation CCD diffractometers means that more laboratories once again have routine access to Cu *K*α radiation, thereby allowing more successful absolute structure determinations to be carried out for light-atom structures. Therefore, the results of crystal structure determinations which demonstrate new successes and remaining limitations in the field of absolute structure determination are of particular interest.

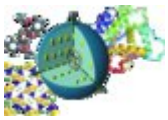
Papers that have been accepted for publication between 1 January 2011 and 30 September 2012 will be included in the issue. Authors interested in contributing new papers for this virtual issue only need to submit their papers to *Section C* in the usual way in the coming months. These will be published shortly after they are accepted, as normal, and then collated into the virtual issue towards the end of the year. Authors do not need to make any special request to have their paper included. To submit an article, go to http://journals.iucr.org/c/services/submit.html.

MEETING REPORT

Erice Schools of Crystallography

Erice, Italy, June 2–12, 2011
www.crystalerice.org/

Electron Crystallography – New Methods to Explore Structure and Properties of the Nano World





Electron Crystallography school participants.
The course was held in parallel to 'The Power of Powder Diffraction' with 90 total participants from 25 countries, and included 38 lectures, 9 demo talks, 16 lab courses and 25 poster presentations. The school had three major goals.

1) To provide a strong background on crystallography in general and electron crystallography in particular.

Since the participants' backgrounds were diverse, basic lectures on crystallography and electron microscopy proved to be extremely helpful. Leaders in the field gave lectures on the fundamentals of crystallography, electron diffraction theory and the theory of image formation in the electron microscope, as well as the construction of electron microscopes. (M. Gemmi, Italy; C. Giacovazzo, Italy; K. Tsuda, Japan; L. Meshi, Israel; L. Marks, USA; J. Jansen, Netherlands; D. van Dyck, Netherlands; J. Paul Morniroli, France; J. Hadermann, Belgium; and R. Dinnebier, Germany).

Demo talks and lab sessions (T. Gorelik, Germany; E. Mugnaioli, Germany; P. Müller, USA; and G. L. Cascarano, Italy) provided insight into software for data analysis, processing and interpretation.

2) To introduce students to techniques for data acquisition and processing.

New technical developments (O. Krivanek, USA; U. Kaiser, Germany; J. Pieter Abrahams, Netherlands) as well as new methodologies (P. Oleynikov, Sweden; S. Rubino, Sweden; C. Koch, Germany; U. Kolb, Germany) were covered. A series of talks on established methods and the possibilities to improve their precision were given (S. Hovmöller, Sweden; S. Nicolopoulos, Belgium; K. Tsuda, Japan; Y. Zhu, USA; A. Avilov, Russia; M. Gemmi, Italy; L. Marks, USA; J. Jansen, Netherlands)

3) To cover different approaches for structure solution and derivation of structure-property relationships.

The structure solution lectures were held jointly with the powder course (C. Giaccovazzo, Italy; C. Gilmore, Scotland; L. Palatinus, Czech Rep.; K. Shankland, Britain; C. Bärlocher, Switzerland; M. U. Schmidt, Germany), giving the participants of both courses a chance to gain a deeper understanding of complementary scientific fields. Additional presentations were given on specialized methods and algorithms to achieve structural information (F. Chukovskii, Russia; A. Stewart, Germany). The course covered crystallography of inorganic and organic materials, aperiodic structures and proteins (M. van Heel, Britain; J. P. Abrahams, Netherlands; and M. U. Schmidt, Germany). The investigation of structure-property relationships was covered by methods of direct measurements as well as by indirect analysis. (S. Rubino, Sweden; R. Dunin-Borkowski, Germany; M. Hytch, USA).

The lecturers included young and promising scientists as well as leaders in the field. This and the high variety of topics gave all scientists, lecturers and students the opportunity to learn from one another and to gain new ideas. The results of a questionnaire distributed to all participants gave a very positive score of 90 for the meeting overall and nearly 82 for the workshop component.

Electron Crystallography Prizes

Poster Prize Winners

Dmitri Batuk (U. of Antwerp, Belgium)
Maria Batuk (U. of Antwerp, Belgium)
Shmuel Samuha (Ben Gurion U., Israel)

Special Mention

Tom Willhammar (Stockholm U., Sweden), Irina Andrusenko (U. of Mainz, Germany), Miguel Avalos (Inst. Potosino de Investigacion Cientifica y Tecn., Mexico), Mariana Klementova (Inst. of Physics, Czech Rep.), Wilder Carrillo-Cabrera (Max Planck Inst., Germany) and Christoph Gammer (U. of Wien, Austria)

Lodovico Prize

Song Bo (Delft U. of Technology, The Netherlands)

Special Mention

Lotnyk Andriy (U. of Kiel, Germany) and Pallewatta A. Pramod (Risø Nat'l Lab. for Sustainable Energy, Denmark)

The Power of Powder Diffraction





Participants in the Power of Powder Diffraction school.
This intensive course involved 78 participants and 26 speakers from 30 countries. The program included 39 lectures, 9 software demonstrations and 12 workshops. Lecture notes, including written contributions by the invited speakers, poster abstracts and photos of all contributors, were distributed to everyone upon arrival in Erice. All this was backed up by excellent IT facilities and support.

This comprehensive course on the diverse field of powder diffraction covered fundamentals, instrumentation at the frontiers, structure solution, challenging systems, complementary methods, imperfect materials, quantitative phase analysis, textured systems and future trends. Instrumentation was covered from the basic laboratory level through the facility (synchrotron and neutron) level, with a view to highlighting the various levels at which powder diffraction is performed and the scientific opportunities that such diversity affords.

The speakers presented complex material in ways accessible to an audience with a wide range of expertise and experience. Lectures were reinforced by demonstration sessions and follow-up workshops. Participants were encouraged to bring their own laptops and install the relevant software/data, and learn enough to work with the software long after the close of the meeting. Most speakers were present for the duration of the course for informal discussions. Groups of participants could meet with a designated tutor (speakers) for lunch.

Several awards were made for the best poster presentations and the main ('Lodovico') award was given to Paul Smart (U. of Sheffield), for his questions and contributions to discussions over the duration of the course.

More than 98% of attendees expressed the feeling that there should be another meeting along similar lines, held within the next 6 years. Various suggestions for improvements at future meetings were also received, particularly on maximizing the value of the workshop component.

Powder Diffraction Prizes



Erice 2011 Schools of Crystallography award winners with school directors Louisa Meshi and Ute Kolb (Electron Crystallography), Kenneth Shankland and Bill David (Powder Diffraction), Simon Billinge (a judge of the poster prize), Paola Spadon and Annalisa Guerri.

Poster Prizes

Andrew K. Inge (Stockholm U., Sweden)
Dubravka Sisak (ETH, Zurich, Switzerland)
Martina Vrankic (Rudjer Boskovic Inst., Croatia)

Special Mention

Niels Bindzus (Aarhus U., Denmark), Tanja Gnutzmann (BAM Federal Inst. of Mat. Res. & Testing, Germany), Marcin Oszajca (Jagiellonian U., Poland), Jasminka Popovic (Rudjer Boskovic Inst., Croatia) and Casper Ibsen (Aarhus U., Denmark).

Lodovico Prize

Paul Smart, University of Sheffield, Sheffield, UK

Special Mention

Saul Lapidus (SUNY Stony Brook, USA), Giulio I. Lampronti (U. of Bologna, Italy), Paolo P. Mazzeo (U. of Bologna, Italy), Mark Senn (U. of Edinburgh, UK)

Annalisa Guerri

MEETING REPORT

8th International School on Crystallography and X-ray Diffraction

Havana, Cuba, November 21–25, 2011



Synchrotron light facilities all over the world continue to provide access to a growing number of researchers from different scientific fields. The 8th International School on Crystallography and X–ray Diffraction held in Havana Cuba in November 2011 was designed to increase the number of scientists in our region that can make use of available synchrotron facilities in their research and to promote postgraduate studies in the field. The school addressed the subjects of 'Principles and Application of Synchrotron Light Sources' and 'Basic Principles of Crystallography'. It brought together 25 students from Ecuador, Venezuela, Vietnam and several Cuban scientific institutions. The invited speakers were: P. Paufler (Inst. f. Strukturphysik, Technische U., Dresden, Germany), Juan Rodriguez-Carvajal (Inst. Laue-Langevin, Grenoble, France), Ernesto Estevez Rams (IMRE – U. of Havana, Cuba), Jasper Plaisier (ELETTRA Synchrotron, Trieste Italy), Eduardo Granado (LNLS, Campinas, Brazil) and Gema Martinez-Criado (ESRF, Grenoble, France).

This school was sponsored by the International Union of Crystallography (IUCr), the Latin American Center of Physics (CLAF), IMRE and the Physics Faculty of Havana U., and received support from Colegio U. San Gerónimo, Habana Vieja, Cuba.

Arbelio Penton Madrigal

OBITUARY

Gabriel Germain (1933-2011)



Gabriel Germain was born in December 1933 in Salles (Chimay), a small village close to the French border. He died in the house where he was born, as he often said he would like to do. He obtained his Chemistry degree at the U. of Louvain, where he began his teaching career.

In 1964 Gabriel went to the U. of Manchester, Institute of Science and Technology, to work with Michael Woolfson developing methods for solving crystal structures. He was accompanied by his wife Marguerite and their children Marc and Anne. His first challenge was to acclimatize himself to life in the UK. When in response to his query he was told that there are no regular deliveries of beer to homes in the UK he seemed genuinely astonished!

His collaboration with Woolfson was not on direct methods but involved deriving phase information from the Patterson function. Up until 1964 sign relationships were being used to solve small centrosymmetric structures, but in 1964 Isabella and Jerome Karle extended a method, proposed by William Cochran, in which signs were represented by letter symbols. The Karles used this technique, which they called 'symbolic addition', to solve both centrosymmetric and non-centrosymmetric structures. In 1965 Woolfson and Germain moved to York, where their first project was to design a computer-based multisolution symbolic-addition method to solve centrosymmetric structures. The computer at York was primitive by today's standards, an Elliott 4130 with a 32K processor. Gabriel's skill in using these limited facilities was remarkable – not a byte was unused and not a byte was wasted. The resultant program *LSAM* (Logical Symbolic Addition Method) was very successful and soon they moved on to design a multisolution method for non-centrosymmetric structures, assisted by Peter Main who moved to York in 1967. The resultant program *MULTAN*, which used a novel approach to structure solution, was first distributed in 1971 and, for many years most small non-centrosymmetric structures worldwide were solved by its use.

By this time Gabriel had returned to Belgium, but he continued his collaboration in the development of *MULTAN*. In 1969 during a five-week workshop held in Paris, he and Peter Main could exploit the more powerful computer made available by CECAM (Centre Européen de Calcul Atomique et Moléculaire) to set up an improved version of *MULTAN*. The collaboration was effectively ended in 1986 with the distribution of *MULTAN1987*.

Gabriel published more than 400 papers which garnered more than 10,000 citations. He collaborated with crystallographers throughout Europe, South America and Africa, helping them to phase challenging crystallographic problems. In Spain alone he collaborated with more than 30 researchers from 10 different universities and research centres.

In 1984 he was awarded the Doctor *honoris causa* by the Universitat Autònoma of Barcelona. He spent a sabbatical year (1989) in the crystallography department there and was a regular visitor to the department until his retirement in 1998.

Many crystallographers enjoyed the warm hospitality of Gabriel and his wife Marguerite in their home where pleasant after dinner soirées were spent discussing many subjects in front of a Chimay or a Stella Artois beer.

Gabriel was a reserved person, with a preference for doing science, producing useful software or solving difficult crystal structures. He preferred interpersonal relations to large meetings and he enjoyed tutoring young people on the subtleties of the practical solution of the phase problem in resistant cases.

Davide Viterbo, Michael Woolfson and Juan Piniella