INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

Volume 18 · Issue 4

Collected archival edition
Original article text and available illustrations

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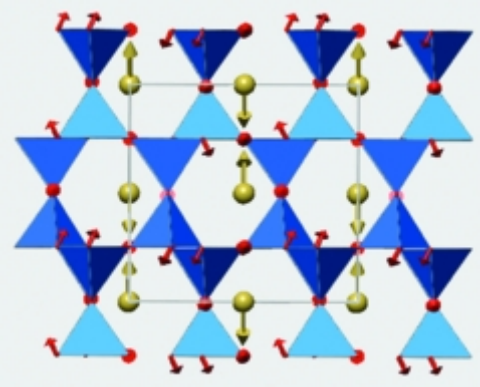
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IUCR JOURNALS NEWS

Mode crystallography of distorted structures

Acta Cryst. (2010). A66, 558-590 (doi.org/10.1107/S0108767310016247)



Antiferrodistortive primary distortion mode (from a parent $P6_322$ structure) present in the $P2_1$ structure of $SrAl_2O_4$.

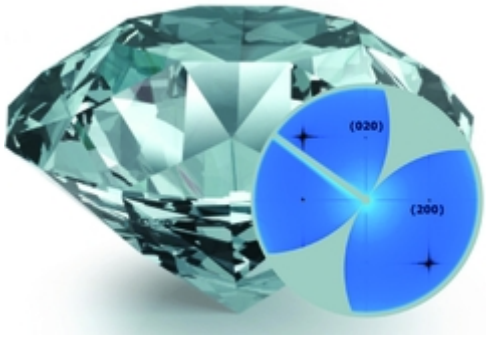
Many crystals can be considered distortions of configurations of higher symmetry. Their description in terms of symmetry-adapted modes has many advantages. Free computer tools that closely follow crystallographic conventions are now available for a straightforward application of this approach. The methodology is reviewed and several examples illustrate its possibilities, as for instance, detection of hidden correlations, identification of fundamental and marginal degrees of freedom, reduction of the number of positional parameters, comparison of structures, detection of false refinement minima, and analysis of thermal behaviour or phase diagrams.

J. M. Perez-Mato, D. Orobengoa and M. I. Aroyo

IUCR JOURNALS NEWS

Symmetry of platelet defects in diamond: new insights with synchrotron light

Acta Cryst. (2010). B66, 493-496 (doi.org/10.1107/S0108768110031071)



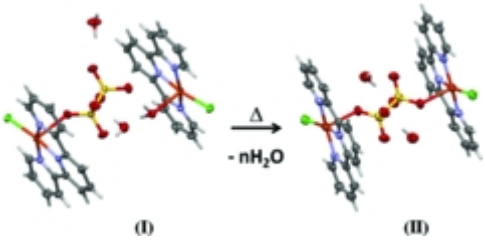
Nearly 98% of natural diamonds are of type *Ia*. They contain up to 0.3% nitrogen, mainly associated with planar defects, called platelets. As all the platelets are coherently integrated into the single-crystal diamond matrix, their assembly can be treated as a twinned composite crystal. Three-dimensional mapping of rod-like diffuse scattering from *Ia* diamonds allowed us to identify the periodicity ($\sqrt{8}a_0 \times \sqrt{1/2}a_0 \times -0.55a_0$) and some symmetry elements of the platelets. Our findings should guide further work to solve the structure of these defects.

A. Bosak, D. Chernyshov, M. Krisch and L. Dubrovinsky

IUCR JOURNALS NEWS

Crystal-to-crystal transformation upon dehydration of a copper(II) 2,2′:6′,2″-terpyridine complex

Acta Cryst. (2010). C66, m343-m347 (doi.org/10.1107/S0108270110041090)



The crystal-to-crystal transformation of the ionic copper(II) terpyridine complex (I) into the binuclear complex (II).

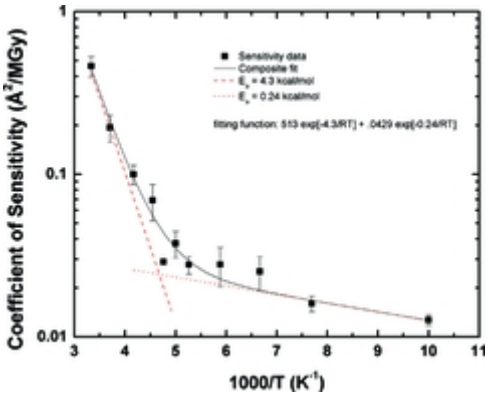
Crystal-to-crystal transformations are not uncommon and many are the result of dehydration of transition metal complexes. By carefully heating the ionic copper(II) terpyridine complex, (I), the coordinated water molecule of the cation could be eliminated, leaving a free coordination site on the metal. This was then filled by a suitably positioned O atom of the thiosulfite ligand of the anion, and resulted in the transformation of the ionic complex (I) into a centrosymmetric binuclear complex (II).

L. Schmitt, G. Labat and H. Stoeckli-Evans

IUCR JOURNALS NEWS

Glass transition in thaumatin crystals revealed through temperature-dependent radiation-sensitivity measurements

Acta Cryst. (2010). D66, 1092-1100 (doi.org/10.1107/S0907444910035523)



The temperature-dependence of radiation damage to thaumatin crystals is reported, revealing two regimes of thermally activated behavior. At temperatures above ~200 K the activation energy indicates that radiation damage is dominated by diffusive motions, but below ~200 K the activation energy is similar to those reported for radiation damage to a variety of solvent-free small-molecule organic crystals. These results also suggest that data collection at $T \approx 220$ K may provide a viable alternative for structure determination when cooling-induced disorder at 100 K is excessive.

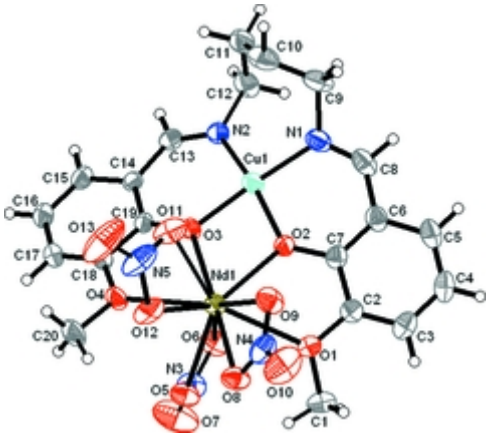
M. Warkentin and R. E. Thorne

IUCR JOURNALS NEWS

{μ2-6,6′-Dimethoxy-2,2′-[butane-1,4-diylbis(nitrilomethylidyne)]diphenolato}-trinitratocopper(II)neodymium(III)

{μ_2-6,6′-Dimethoxy-2,2′-[butane-1,4-diylbis(nitrilomethylidyne)]diphenolato}-trinitratocopper(II)neodymium(III)

Acta Cryst. **(2010). E66, m1423 (doi.org/10.1107/S1600536810040833)**



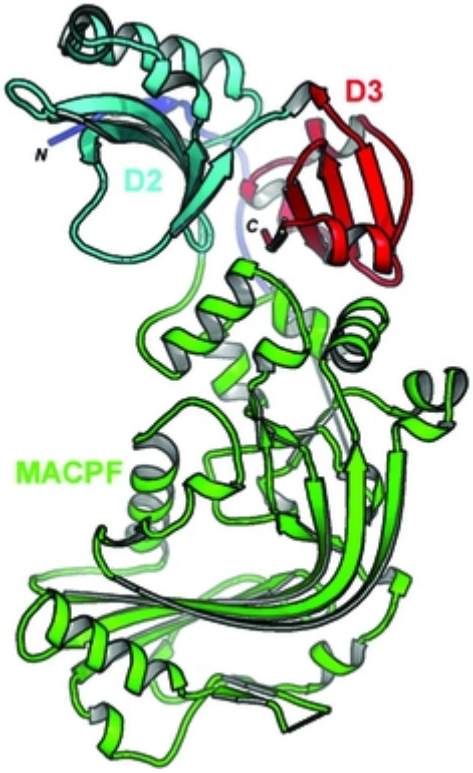
The molecular structure of the title complex is shown in the figure. The Cu^{II} ion is coordinated in a distorted square-planar environment by two O atoms and two N atoms of a tetradentate Schiff base ligand. The Nd^{III} ion is ten-coordinated by three bis-chelating nitrate groups and four O atoms of the Schiff base ligand. The atoms of one of the nitrato ligands are disordered over two sets of sites, with refined occupancies of 0.567 (13) and 0.433 (17).

J.-C. Xing, X.-G. Cui, B. Zhang and W.-Z. Li

IUCR JOURNALS NEWS

Structure of a membrane-attack complex/perforin (MACPF) family protein from the human gut symbiont Bacteroides thetaiotaomicron

Acta Cryst. **(2010). F66, 1297-1305 (doi.org/10.1107/S1744309110023055)**



Structure of BT_3439.

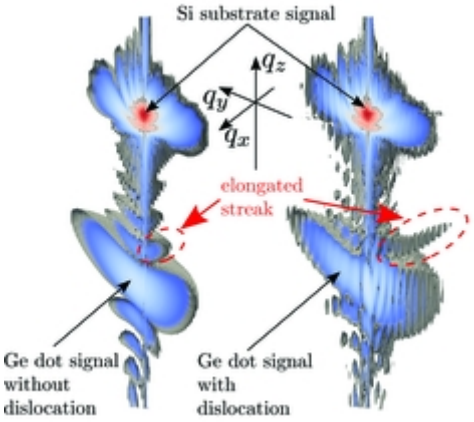
MACPF proteins are important in human immunity and in virulence of pathogens due to their ability to compromise membrane integrity by forming transmembrane pores. The structure of an MACPF-domain-containing protein BT_3439, a potential toxin from a gut symbiont, contains an MACPF domain and two novel C-terminal domains (D2, D3) that have not been observed in previous MACPF structures. The MACPF proteins from Bacteroidetes were likely acquired independently from a eukaryotic origin via horizontal gene transfer to adapt better to the host environment.

Q. Xu et al.

IUCR JOURNALS NEWS

Algorithms for the calculation of X-ray diffraction patterns from finite element data

J. Appl. Cryst. (2010). 43, 1287-1299 (doi.org/10.1107/S0021889810032802)



Simulated 3D intensity distribution of a coherent and a dislocated quantum dot computed with one of the developed algorithms.

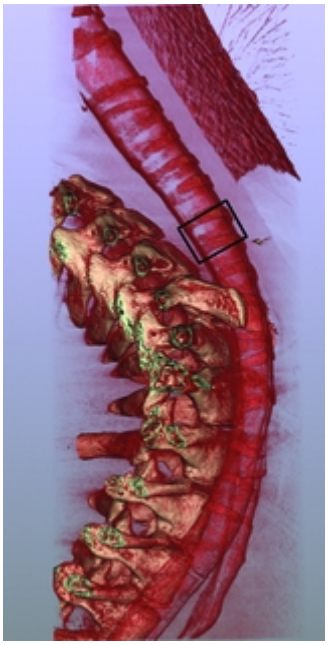
The use of CCD detectors in diffraction experiments allows the collection of 3D data sets containing much more information than scans in 1 or 2 dimensions. This, however, dramatically increases the demands on data analysis, which is based on a simulation of the scattered intensity from finite element modeling of the atomic displacements in a sample. We developed algorithms for the efficient calculation of such 3D diffraction data. As application examples the quantitative interpretation of diffraction data from dislocation arrays and quantum dots is presented.

E. Wintersberger, D. Kriegner, N. Hrauda, J. Stangl and G. Bauer

IUCR JOURNALS NEWS

A new technique to examine individual pollutant particle and fibre deposition and transit behaviour in live mouse trachea

J. Synchrotron Rad. (2010). 17, 719-729 (doi.org/10.1107/S0909049510028451)



3D rendering showing the region of the mouse trachea adjacent to the spine where particle and fibre behaviour was examined.

Unless cleared by airway defenses deposited pollutants can remain and affect lung health. Synchrotron phase contrast imaging was used to examine pollutant particle behaviour after deposition onto the tracheal airway surfaces of live mice. Each particle and fibre looked and behaved differently on the airway surface, suggesting the interaction between individual particles and the airway may depend on the particle type and size. This method should provide a novel approach to monitoring the acute effects of respired particles on airway function.

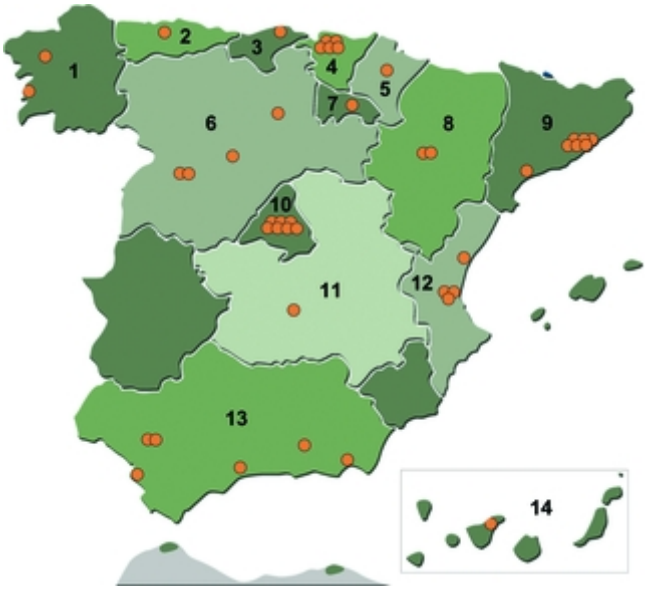
M. Donnelley, K. K. W. Siu, K. S. Morgan, W. Skinner, Y. Suzuki, A. Takeuchi, K. Uesugi, N. Yagi and D. W. Parsons

SPECIAL REPORT

Crystallography in Spain

Crystallographers in Spain

Continued from Volume 18, Number 3



Crystallography groups in Spain. Orange circles show their approximate location. Numbers mean regional references only used in the text.

Crystallographers in Spain belong to one or more of the following organizations: the European Crystallographic Association (ECA) and the Group for Crystallography and Crystal Growth (GE3C), a group associated with the Spanish Royal Society of Chemistry (RSEQ) and the Spanish Royal Society of Physics (RSEF). Other Spanish associations related to crystallography include the Spanish Association of Synchrotron Users (AUSE, http://bit.ly/c1S3j7) and the Spanish Association for Neutron Techniques (SETN, http://bit.ly/aI5Ana). The Spanish Committee of Crystallography is the official Spanish representative to the IUCr.

Teams of Spanish crystallographers are concentrated in the regions described below. An updated list of groups in Spain can also be found at www.xtal.iqf.csic.es/Cristalografia/ (in Spanish and English).

1. Galicia

Galicia is an Autonomous Community in northwestern Spain with an ancient Celtic culture (5th Century BC). It became a Roman province (Gallaecia) in 197 BC, one of the first Catholic kingdoms in 449.



The GIQIMO group



C-terminal fragment of avian reovirus σC fiber protein.

The Grupo de Investigación de Química Molecular y Estructural (GIQIMO), at the U. of Santiago de Compostela, was developed by A. Castiñeiras (qiac01@usc.es) in 1980 after his stay at the Dept. of Crystallography and Structural Biology of the Spanish National Research Council (CSIC) in Madrid (see below, No. 9). Their research concerns magnetic materials, bioinorganic chemistry, structural chemistry, crystal engineering and supramolecular structures (http://bit.ly/aeHKbf).

At the U. of Santiago de Compostela the research team of A. Llamas (antonio.llamas@usc.es) engages in research projects in Inorganic, Organic and Biochemistry and is developing macromolecular crystallographic research on adenovirus proteins, viral fibers, dehydroquinase-inhibitor drug complexes and cyclic peptides (GramS analogs), (http://bit.ly/cGJa6X). The Universities of Vigo and Coruña maintain X-ray diffraction equipment as general service units for their universities (http://bit.ly/eVsMxW and http://bit.ly/9zwfIV, respectively).

2. Asturias

Asturias, on the north coast of Spain facing the Cantabrian Sea, has been occupied by humans since the Lower Paleolithic era. It has cave paintings and megaliths from the Bronze Age. There were Celtic inhabitants in the Iron Age, Romans from 29 to 19 BC, Visigoths from the 6th to the 8th century and then the Moors invaded. The lands along the northern coast were never fully part of Islamic Spain and became a refuge for Christian nobles. In 722, a *de facto* independent kingdom was established, the Regnum Asturorum, which was to became the cradle of the incipient Reconquest.

The Dept. of Physical Chemistry at the U. of Oviedo has one of the most active Spanish crystallographic teams in Asturias. It was established in the 80s by F. Beltrán and S. García-Granda (sgg@uniovi.es) for study of molecular structure and properties, automatic determination, QSAR and QSPR modeling, and chemical crystallography. S. García-Granda is currently the President of the European Crystallographic Association (ECA) (http://bit.ly/9viBu4). The Group on Crystal Growth and Experimental Aquatic Geochemistry at Oviedo U. is a multi-departmental team supported by the European Commission to study the dissolution and precipitation rates of solid solutions. Groups from six European countries participate in this project. The Spanish team is headed by M. Prieto (mprieto@geol.uniovi.es) (http://bit.ly/anZmfz). In the Dept. of Physics of Oviedo U., J. A. Blanco (jabr@uniovi.es) and P. Gorria (pgorria@uniovi.es) study magnetic materials with neutron diffraction.

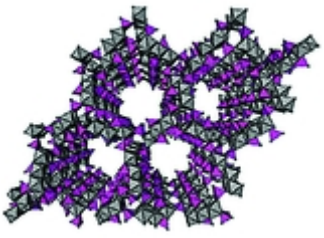
3. Cantabria

Cantabria is one of the richest regions in the world in archaeological sites from the Upper Paleolithic period. Paintings in the cave of Altamira date from 16,000 BC.

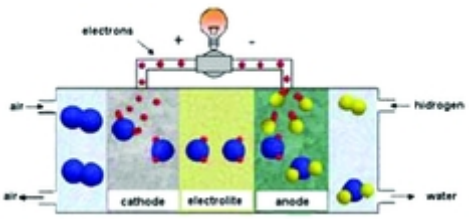
In 1974 the magnetic materials group of Cantabria U. headed by J. C. Gómez Sal (jose.gomezsal@unican.es) published the first magnetic structure from Spain and developed collaborations with the neutron and X-ray communities at the ILL. The activities of the group, with J. R. Fernandez (jesus.rodriguez@unican.es) and L. F. Barquín (barquinl@unican.es), include crystallization, crystal and magnetic structures and small-angle diffraction of metals and nanocrystals (http://bit.ly/ceXiJZ). In the High Pressure and Spectroscopy Group, F. Rodriguez (fernando.rodriguez@unican.es) examines the structures of insulators under extreme conditions (http://bit.ly/b0j7BK).

4. The Basque Country

The Basque Country in the western Pyrenees spans the border between France and Spain. Although little is known about the prehistory of the Basques, several Basque archaeological sites provide evidence for continuity from Aurignacian times to the Iron Age. Some of the same people appear to have continued to inhabit the area for thirty millennia.



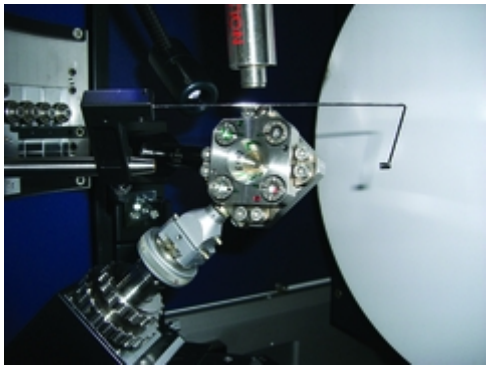
Structural porosity in arsenates of transition metals with organic molecule and ammonium cations.



Scheme of a solid oxide fuel cell.

The Dept. of Mineralogy and Petrology of the U. of the Basque Country (UPV/EHU http://bit.ly/92zVzg), is headed by K. Urtiaga (karmele.urtiaga@ehu.es), and M. I. Arriortua (maribel.arriortua@ehu.es) is currently Director of the General Services for Research of the UPV/EHU for the entire university (http://bit.ly/cFitTW). Research targets are multifunctional systems for environmental and energy applications including zeotypic materials. Microporous inorganic frameworks that can bind organic molecules are being studied for potential use for gas separation, as molecular sieves or in catalytic processes. The group is also attempting to optimize the performance of solid oxide fuel cells (SOFC) via their full characterization before, during and after operation. The long-term goals are to achieve cost-effective processing techniques, reduce operating temperatures and find inexpensive stable and durable materials.

The Dept. of Inorganic Chemistry (UPV/EHU) directed by P. Román (pascual.roman@ehu.es) has three major projects on two campuses. Laminar and tubular magneto-resistant phosphate transition metals, mixed oxides of technological interest and molecular magnetic materials are being studied by T. Rojo (teo.rojo@ehu.es); the chemistry of polyoxometalates and organic-inorganic hybrid systems is led by J. M. Gutiérrez-Zorrilla (juanma.zorrilla@ehu.es); and studies of the magnetic behavior of polynuclear complexes with polyfunctional organic ligands are co-directed by P. Román (pascual.roman@ehu.es) and A. Luque (antonio.luque@ehu.es) (www.ehu.es/qi/).



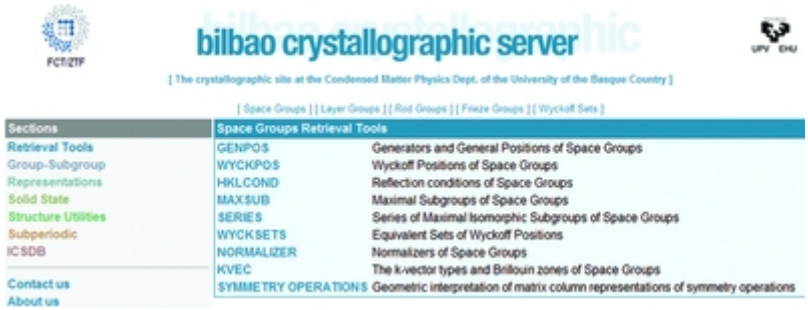
The Ahsbahs-type diamond cell mounted in Bilbao on the IPDS-2T diffractometer (Stoe & Cie GmbH, Darmstadt, Germany).

The Group of Structural and Dynamical Properties of Solids, headed by J. M. Pérez-Mato (wmppemam@lg.ehu.es) at the Dept. of Condensed Matter Physics of the Basque Country U. (UPV/EHU) in Bilbao (I. Aramburu, M. I. Aroyo, L. Elcoro, I. Etxebarria, K. Friese, A. Grzechnik, J. Igartua, G. Madariaga and F. J. Zúñiga) focuses on structural and lattice dynamics of functional materials, phase transitions in inorganic and molecular crystals, mathemathical crystallography, nonconventional crystallographic methods, thermal properties, aperiodic crystals, high-pressure crystallography and *ab initio* studies of ferroic materials.



Three-dimensional atomic domain describing the atomic positions of a subset of atoms of an icosahedral quasicrystal, within a 6-D super-space refined model.

The UPV/EHU was founded in 1969, as a result of the teaching skills and the contagious scientific enthusiasm of J. Eugenio Iglesias. His students F. Javier Zúñiga and J. M. Perez-Mato joined the Physics Dept. to form the nucleus of the group that studied phase transitions, incommensurate phases and aperiodic crystals. In 1991 the group organized an 'International workshop on methods of structural analysis of modulated structures and quasicrystals' in Lekeitio (Spain) which influenced the development of the field. The team of physicists had a natural affinity for studies of structural thermal behavior and methods of analysis of aperiodic crystals. Recently, scientists with mineralogical and chemical backgrounds (K. Friese, A. Grzechnik) have joined the group, fostering multidisciplinary work.



Heading of the Bilbao Crystallographic Server, a popular webpage with online computer tools for crystallographic analysis.

The Bilbao Crystallographic Server (www.cryst.ehu.es/), directed by M. I. Aroyo, provides free online access to crystallographic databases, computer tools and programs for crystallographers and materials scientists. An international school on the use and applications of this server was organized in 2009. A database of incommensurate structures is being reorganized by G. Madariaga.

The Magnetism and Magnetic Materials Group (UPV/EHU), headed by J. M. Barandiaran García (manub@we.lc.ehu.es), works on nanocrystalline structures and crystallization processes (http://bit.ly/cetJqA). The Biophysics Unit, a joint center of UPV/EHU and the CSIC, headed by F. M. Goñi (felix.goni@ehu.es), was created in 1999 and studies mainly biological membranes. The crystallography group headed by D. Guérin (gbxguxxd@lg.ehu.es) conducts research on membrane protein crystallization, crystallization in lipidic mesophases and virus crystallography (www.unidaddebiofisica.org/).

The Center for Cooperative Research in Biosciences (CIC bioGUNE), headed by J. M. Mato, is a non-profit biomedical research organization founded in 2002 by the Dept. of Industry of the Basque Government and opened in 2005 (www.cicbiogune.com). The Structural Biology Unit at the CIC bioGUNE is composed of four groups. The group headed by A. Martínez de la Cruz (amartinez@cicbiogune.es) focuses on cystathionine β-synthase domains and is part of the Spanish Ion Channel Initiative, a multidisciplinary cooperative headed by A. F. Montiel from the U. Miguel Hernández in Elche, Spain. A group headed by L. Malinina (lucy@cicbiogune.es) is focused on protein complexes with RNA and lipids related to neurodegenerative diseases. The leader of the third group is A. Hierro Ayuela (ahierro@cicbiogune.es), whose research interest is intracellular trafficking processes. N. G. A. Abrescia (nabrescia@cicbiogune.es) leads the fourth group, using crystallography to study virus assembly mechanisms and archaeal transcription machinery (http://bit.ly/a4DTF4).

5. Navarre

In 824, Iñigo Arista was chosen King of Pamplona, laying a foundation for the Kingdom of Navarre, which at its zenith covered the area of the present-day Navarre, the Basque country, La Rioja, and parts of modern Cantabria, Castile, León and Aragon. The army of Navarre fought in the battle of Las Navas de Tolosa in 1212, after which the Muslim conquests on the Iberian Peninsula were slowly reduced to a small territory in the south. In 1515, Navarre south of the Pyrenees was absorbed into the Kingdom of Spain and Navarre north of the Pyrenees came under French rule.

In the Dept. of Physics of the Public U. of Navarre, V. Recarte (recarte@unavarra.es) and I. P. de Landazabal (ipzlanda@unavarra.es) study structural transformations and magnetic properties of ferromagnetic alloys with shape memory, as part of the Physical Properties and Applications of Material Group (http://bit.ly/bfT7fT).

6. Castile and León

Ferdinand III of Castile, later canonized, united the Crowns of Castile and Leon in 1231. The medieval Cortes of León is one of the earliest ancestors of Europe's parliaments. The Cortes of León of 1188, called by Alfonso IX, is one of the earliest documented gatherings of the estates in which commoners of the cities and towns are represented beside the clergy and nobility as counselors to the monarch.



From left to right: J. M. de Pereda, E. Ortega, N. Alonso and M. Gómez

Macromolecular crystallography in the vast region of Castile and León is represented by the Structural Biology Group at the Cancer Research Center (CIC), coordinated by both the U. of Salamanca and the Spanish National Research Council (CSIC). The group was established in 2003, when J. M. de Pereda (pereda@usal.es) joined the CIC after post-doc training in Leicester, UK, and San Diego, CA. The group applies protein crystallography to study cell-adhesion and signaling proteins, such as the integrin family of receptors. Since this is the first laboratory devoted to macromolecular crystallography in the Castile and León region, the training of young students and collaboration with local non-crystallography laboratories are two major aims of the group (http://xtal.cicancer.org).

Three universities in the Castile and León region have service units for X-ray diffraction studies. U. of Salamanca, directed by F. Sanz (sdrayosxr@usal.es), (http://bit.ly/b1W7Ov); the U. of Burgos headed by J. J. Delgado (jdelgado@ubu.es), (http://bit.ly/bmx8aB), and U. of Valladolid, headed by F. Rull (rull@fmc.uva.es).

7. La Rioja

La Rioja is known for its wonderful wines. The Oja river ('rio') that flows through this region gives the name to this province. The U. of La Rioja has a central diffraction unit run by J. Berenguer (jesus.berenguer@unirioja.es).

8. Aragon

Saragossa is the capital of Aragon in northeastern Spain. James I the Conqueror was the King of Aragon, Count of Barcelona, and Lord of Montpellier from 1213 to 1276. After the marriage of Isabella I of Castile and Ferdinand II of Aragon at the end of the fifteenth century, there was a dynastic union of both crowns and most other kingdoms in Spain. Aragon remained a separate kingdom, with its own laws and institutions, until 1707. At that point Philip V, the first Bourbon king of Spain, consolidated Spain into a more centralized state.

Crystallographic research in this region is to be found in four different groups, three of them belonging to the Inst. of Material Sciences of Aragon, a joint center between the U. of Saragossa and the CSIC, and one involving only the university.



From left to right: Larry Falvello, Milagros Tomás and Francisco Mart&iaute;nez.

The Preparation, Properties and Molecular Solid Transformations Group, headed by L. Falvello (falvello@unizar.es) concerns the preparation and characterization of molecular solids, their properties, dynamical behavior and transformations. (http://bit.ly/aDVwIv). The Coordination Chemistry and Homogeneous Catalysis Dept. of F. J. Lahoz emphasizes coordination chemistry of platinum metal complexes, mainly of Rh, Ir, Ru and Os, organometallic reactivity, and in homogeneous catalysis (lahoz@unizar.es), http://bit.ly/ayrYhD. The Dept. of Physics of Condensed Matter is headed by J. Campo (javier.campo@unizar.es), coordinator of the Spanish Collaborating Research Group at ILL and president of the Spanish Association for Neutron Techniques (SETN), and focuses on molecule-based magnets, neutron scattering and magnetic chirality (http://bit.ly/bXfx5u).

At the Inst. for Biocomputation and Physics of Complex Systems (BIFI) of the U. of Zaragoza, crystallographers R. Hurtado (rhurtado@bifi.es) and M. Martínez (mmartinez@unizar.es) conduct research in biological systems (http://bifi.es/).

9. Catalonia

Catalonia has three official languages, Catalan, Spanish and Aranese. Catalonia was colonized by ancient Greeks and Carthaginians. After the defeat of Carthage by Rome, it became a part of the Roman Empire. Catalonia came under Visigothic rule for four centuries and in the eighth century it came under Moorish control. After the defeat of Emir Abdul Rahman Al Ghafiqi's troops at Tours in 732, the Franks conquered the former Visigoth states. In 795 Charlemagne created the Marca Hispanica, a buffer zone of small kingdoms between the Moors and the Frankish Kingdom where the Catalan culture developed. The counts of Barcelona were Frankish vassals. In 989, Catalonia declared its independence. In 1137, a Count of Barcelona married Queen Petronila of Aragon, establishing the dynastic union of the County of Barcelona with the Kingdom of Aragon that was to create the Crown of Aragon. Catalonia became a maritime power, helping to expand the Crown into the Kingdom of Valencia, the Balearic Islands, and ultimately even Sardinia, Sicily, Corsica, Naples, Athens, the Canary Islands and America.

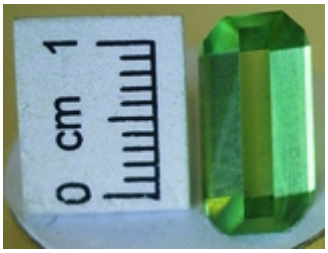
The Dept. of Structural Biology of the Inst. for Molecular Biology of Barcelona, of the CSIC, includes six crystallography laboratories. At the Laboratory of Structural Biology of Proteins, Nucleic Acids and their Complexes, a team headed by M. Coll (mcoll@ibmb.csic.es) study systems related to horizontal gene transfer, DNA translocation and packaging DNA in viral capsids (http://bit.ly/bPCp5E). I. Fita (ifrcri@ibmb.csic.es) leads the Laboratory for Structural Biology of Oxidative Stress Systems (http://bit.ly/ak4m0F). The focus of the Proteolysis Lab, led by F. X. Gomis-Rüth (xgrcri@ibmb.csic.es), is elucidating molecular mechanisms of action of proteolytic enzymes and how bacteria overcome host defenses (http://bit.ly/a0K3uU). M. Solá (msvcri@ibmb.csic.es) leads efforts of the Laboratory of Structural Biology of Organelle Macromolecules to determine structure-function relationships of macromolecules and processes found only in organelles and not in other cellular compartments (http://bit.ly/9UlJkE). The

Laboratory of Crystallographic Methods, led by I. Usón (iufcri@ibmb.csic.es), develops improved methods for macromolecular crystallography, exploiting experimental data and chemical knowledge, deriving general methods to tackle twinning, pseudo-symmetry, anisotropic diffraction, lack of completeness and resolution, *ab initio* macromolecular phasing at medium resolution (implemented in their program *ARCIMBOLDO*), and development of methods exploiting parallel computing in supercomputers and grids (http://bit.ly/aMWbJA). The laboratory of Structural Virology and Large Biological Complexes, headed by N. Verdaguer (nvmcri@ibmb.csic.es), is focused on the structural and functional characterization of different processes in the biological cycle of RNA viruses (http://bit.ly/bp7ihg).



From left to right: Elies Molins, Jordi Rius, Carlos Frontera, Carlos Miravitlles, Amparo Fuertes, Xavier Torrelles, Anna Roig and Judith Oró-Solé at the Institute of Material Sciences of Barcelona.

The Dept. of Crystallography of the Inst. of Materials Science of Barcelona (CSIC) is headed by E. Molins (elies@icmab.es). Crystallographic methodology for single-crystal and powder diffraction data is developed by J. Rius (jordi.rius@icmab.es) and C. Miravitlles (carles.miravitlles@icmab.es); electron-density studies of hydrogen bonds and the relationship between their topology and energy (E. Molins and I. Mata, imata@icmab.es); and magnetic nanoparticles research and crystal engineering of pharmaceutical materials (A. Roig, roig@icmab.es) (http://bit.ly/aJrQHZ). In the Dept. of Magnetic Materials and Functional Oxides, headed by J. L. Garcia-Muñoz (garcia.munoz@icmab.es), high-precision neutron and X-ray diffraction techniques are combined with experimental and theoretical symmetry analyses (http://bit.ly/9Wtw9z). There is additional crystallographic research in the Dept. of Solid State Chemistry (N. Casañ, nieves@icmab.es) (http://bit.ly/dq4vtd).



A single crystal for photonic technology.

In the Dept. of Crystallography, Mineralogy and Mineral Deposits at the U. of Barcelona, S. Galí (gali@ub.edu) and M. À. Cuevas pursue crystallographic studies (mcuevasdiartel@ub.edu) (www.ub.es/cmdm/). In the Biological Macromolecules Group headed by L. Urpí at the Polytechnic U. of Catalonia (lourdes.urpi@upc.edu), the structure of DNA and its interactions with drugs, ions and proteins are under study (http://bit.ly/c53Ep0). FICMA (the group of Physics and Crystallography of Materials), an interdisciplinary research group headed by F. Díaz and M. Aguiló (aguilo@quimica.urv.es) at the U. Rovira i Virgili, located in Tarragona, focuses on the synthesis and structural characterization of new materials for laser and photonic technology and development of optics and photonic devices (http://bit.ly/a4e1jA).

Crystallographic work done at the Inst. of Chemical Research of Catalonia (ICIQ) is done under supervision of J. Benet (jbenet@iciq.es), (http://bit.ly/avdERB). Crystallography carried out at the Crystallography and Mineralogy Unit of the Dept. of Geology of the Autonomous U. of Barcelona is the responsibility of J. F. Piniella (juan.piniella@uab.es) (http://bit.ly/9buGXE).

10. Madrid

Madrid, the capital of Spain, is located at the center of the Iberian Peninsula on the Castilian Central Plateau. This region has been populated since the Lower Paleolithic period. During the Roman Empire it was crossed by two important Roman roads. During the period of the Visigothic Kingdom it was one of the least-populated regions of Al-Andalus, until the 11th century when the Muslim governors created a defensive system of fortresses all across the region with which they tried to stop the advance of the Christian kingdoms of the north. The fortress city of Mayrit (Madrid) was built around 870 AD as a walled precinct for a military and religious community. In 1083, King Alfonso VI of Castile conquered the city of Madrid. It was under the reign of Charles III (1716-1788) that Spain began to be recognized as a nation rather than a collection of kingdoms and territories. He created a National Anthem, a flag and a capital city, with the construction of a coherent network of roads converging on Madrid.

The region of Madrid has, together with the region of Catalonia, the most crystallographic research groups in Spain. They are located in Madrid and its surroundings, including the city of Alcalá de Henares, where Miguel de Cervantes was born. The following departments or crystallography groups are found in Madrid City.



'The Rockefeller', nickname for the Institute of Physical Chemistry 'Rocasolano', one of the research Institutes of the CSIC, the Spanish National Research Council.



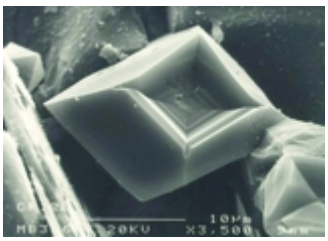
Several members of the Department of Crystallography and Structural Biology, 'at low temperature'.

The Dept. of Crystallography and Structural Biology is located in Madrid, in one of the oldest and most beautiful buildings belonging to the CSIC, the Inst. of Physical-Chemistry 'Rocasolano'. The building was financed by the International Educational Board of the Rockefeller Junior Foundation in 1932 and housed the Inst. Nacional de Física y Química (The National Inst. for Physics and Chemistry) which played a major role in the development of physical chemistry in Spain. Its library is one of the best in its field, with many complete collections of journals, some of which date from the 19th century.

In 1925, B. Cabrera (1878-1945) and his pupil J. Palacios (1891-1970) were responsible for the creation of one of the first Spanish groups of modern crystallography. The department became one of the most important places in Spain to learn crystallography. Today it is one of the best equipped laboratories in Spain, offering wet laboratories and dedicated facilities for protein production, protein characterization, protein crystallization, X-ray diffraction and computing. The department head, A. Albert (xalbert@iqfr.csic.es), is leading a group studying Cellular Stress Response, J. Sanz (xjulia@iqfr.csic.es) and her group are specialists on Carbohydrate Active Enzymes, J. A. Hermoso (xjuan@iqfr.csic.es) is the leader of a group aimed at understanding host-pathogen interactions and new targets to combat antibiotic resistant bacteria (http://bit.ly/9m9vs3), J. M. Mancheño (xjosemi@iqfr.csic.es) is heading projects on enzymes from lactic acid bacteria, and L. Infantes (xlourdes@iqfr.csic.es) is a specialist on molecular docking. These young crystallographers form a dynamic group, and one of the most important pillars of structural biology in Spain, M. Martinez-Ripoll (xmartin@iqfr.csic.es) is a bridge between the previous and the current generations (www.xtal.iqfr.csic.es/). In addition, the department houses the National Associated Centre to the Cambridge Crystallographic Data Center CCDC, distributing free-of-charge sublicenses of CSD for all academic institutions in Spain and Latin American countries. The department also maintains a webpage, in English and Spanish, dedicated to teaching and attracting students to the magical world of crystallography: (http://bit.ly/c8cHaM).

Also in Madrid, and belonging to the CSIC, is the Group of Structural Biology of Proteins which forms a part of the Dept. of Chemical and Physical Biology at the Centre of Biological Research (Centro de Investigaciones Biológicas). The group is headed by G. Giménez, and the research is carried out in three laboratories whose principal investigators are A. Romero (romero@cib.csic.es), C. Vega (cvega@cib.csic.es) and F. Tornero (cftornero@cib.csic.es), http://bit.ly/8Zsp5p.

The National Center for Cancer Research (Centro de Investigaciones Oncológicas, CNIO, in Madrid) has three groups of crystallographers. The Macromolecular Crystallography Group, headed by G. Montoya (gmontoya@cnio.es), is focused on macromolecules involved in oncogenic processes (http://bit.ly/dDdLH); the Cell Signalling and Adhesion Group, headed by D. Lietha (dlietha@cnio.es), probes the mechanisms that regulate focal adhesion kinase at atomic resolution (http://bit.ly/cZn2d8); and S. Ramón (sramon@cnio.es) leads the Structural Basis of Genome Integrity Group, deciphering the structure of the RAG1/2 protein assembly and its regulatory mechanisms and determining the role of recombinase in lymphoid cancer (http://bit.ly/dwOC7r).



Villiaumite (NaF) crystals.

The Dept. of Crystallography and Mineralogy (in the Faculty of Geology) at the U. Complutense of Madrid began in 1956. At that time J. L. Amorós began research on crystal growth and analysis of inorganic and organic materials. Current research involves crystal growth of mineral phases and inorganic compounds at low and high temperature, growth mechanisms of solid solutions from aqueous solutions, diffusing-reacting systems, gemology, epitaxial growth on mineral surfaces, selective chiral symmetry breaking during crystallization, and characterization of geomaterials and other inorganic compounds. The

department, currently headed by J. F. Barrenechea, has over twenty researchers (barrene@geo.ucm.es) (http://bit.ly/avBUbn).

In the Dept. of Inorganic Chemistry I at the U. Complutense, C. Otero (carlos1@quim.ucm.es) leads microstructural characterization of non-molecular crystals with commensurate and/or incommensurate modulated structures (http://bit.ly/aALUdM). The U. Complutense also maintains a General X-ray Diffraction Unit (http://bit.ly/9dXuUc).

The U. Nacional de Educación a Distancia (UNED) in Madrid, together with the Dept. of Geological Engineering of the Polytechnic U. of Madrid, offers a web-based course on crystallography for Spanish-speaking mineralogists known as Cristamine (http://bit.ly/djXrDb).



J. M. Casasnovas' team at the CNB.

At the Autonomous U. of Madrid (AUM), 15 km to north of the city, crystallography groups are found in several departments and research institutes of CSIC. The Dept. of Macromolecular Structures at the National Center of Biotechnology (CNB), a joint center between the Spanish National Research Council (CSIC) and the AUM, includes two groups. The Cell-cell and virus-cell interactions group, headed by J. Casasnovas (jcasasnovas@cnb.csic.es), focuses on receptor-ligand recognition and receptors of the immune system that have been subverted by viruses to enter host cells (http://bit.ly/9tex0T), and the group headed by M. J. van Raaij (markvanraaij@gmail.com) is dedicated to the structural biology of viral fibres.

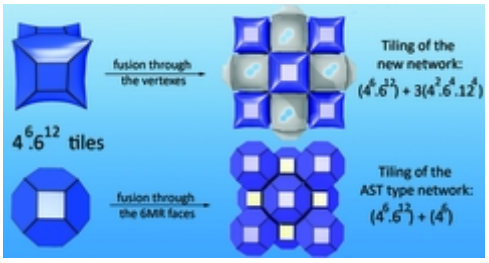


The team of the Crystal Growth Laboratory.

At the Material Physics Dept. of the AUM, the recently established Crystal Growth Laboratory, led by E. Diéguez (ernesto.dieguez@uam.es) participates in national and international projects aimed at crystallizing CdTe and related candidates for gamma-ray detectors for cardiovascular and thyroidal imaging (http://bit.ly/bqaKu9).



Crystallographers at the Department of New Architectures in Materials Chemistry.



Similarity between MOF and zeolite cages.

The Dept. of New Architectures in Materials Chemistry, belonging to the Inst. of Material Sciences of Madrid (CSIC) and located on the AUM campus, is led by E. Gutiérrez-Puebla (egutierrez@icmm.csic.es) and Á. Monge (amonge@icmm.csic.es), who work on the design, synthesis and structure determination of new micro- and nanoporous materials with multifunctional properties (sorption, heterogeneous catalysis, conductivity and optics) and the synthesis of aromatic systems with electrooptic properties (http://bit.ly/bGyavs). In the Dept. of Energy, Environment and Sustainable Technologies at the same Inst. of Material Sciences of Madrid, J. H. Velasco (hernandez-velasco@hmi.de) and J. A. Alonso (ja.alonso@icmm.csic.es) work on new materials using both X-ray and neutron powder diffractometry, and A. Landa (landa@icmm.csic.es) and P. Herrero (pherrero@icmm.csic.es) are active in electron diffraction.



The team of the Structural Chemistry Group at the University of Alcalá.

In 1990, P. Gómez-Sal (pilar.gomez@uah.es) founded the Structural Chemistry Group in the Dept. of Inorganic Chemistry of the U. of Alcalá, where the current activities of A. Martin, M. E. G. Mosquera and others include the synthesis and single-crystal study of organometallic compounds, dendrimers, organometallic polymers and metal-organic frameworks.

11. Castile-La Mancha

Although La Mancha is a windswept, battered plateau, it remains a symbol of the Spanish culture with its sunflowers, mushrooms, olive trees, windmills and Manchego cheese. Castile-La Mancha traces back to the Muslim Taifa of Toledo, which was taken by Alfonso VI from the Muslims in 1085. The Battle of Las Navas de Tolosa (1212) hastened the decline of the Almohad Dynasty. Four centuries later, in 1605, Cervantes' Don Quixote gave the world a lasting picture of La Mancha.

Crystallographic activity is found in several groups belonging to the Dept. of Inorganic Chemistry of the U. of Castile-La Mancha, but mainly in the Group of Organometallic Chemistry and Catalysis, where the crystallographic work is headed by M. I. López (mabel.lopez@uclm.es) (http://bit.ly/csPCpp).

12. Valencia

James I of Aragon led colonization of the Islamic taifas with Aragonese and Catalan people in 1208 and founded the Kingdom of Valencia in 1238. In 1707, King Philip V of Spain subordinated the Kingdom of Valencia and the counties of the former Crown of Aragon.

The Molecular Science Inst. of U. of Valencia has two very active research groups (http://bit.ly/b9NRfN, http://bit.ly/cgTST8) working on structural chemistry, but the crystallographic work is made by other Spanish laboratories. The Dept. of Geology of the U. of Valencia has a group led by J. M. Amigó (jose.m.amigo@uv.es) working on crystallography and mineralogy (http://bit.ly/9rL2wp). In the Dept. of Inorganic Chemistry, three-dimensional structures of organometallic compounds are determined by M. Sanau (mercedes.sanau@uv.es). The Organic Crystal Engineering Group, in the Dept. of Organic Chemistry, headed by C. Rodríguez de Arellano (Carmen.Ramirezdearellano@uv.es), pursues structural studies of organometallic organofluorine compounds and modified peptides (http://bit.ly/aKG5dP).



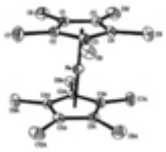
The team of Rosa Llusar at the University Jaume I.

In the Dept. of Inorganic and Organic Chemistry of the U. Jaume I in Castellón de la Plana (north of Valencia), Vicente Esteve (estevev@qio.uji.es) conducts powder diffraction analysis. The Molecular Materials research group of this university, headed by Rosa Llusar (Rosa.Llusar@qfa.uji.es) of the Dept. of Chemistry, Physics and Analytics, is active in single-crystal diffractometry using the equipment of a general service unit of this university (http://bit.ly/bXZQNt).

Macromolecular crystallography is conducted at the CSIC Inst. of Biomedicine in Valencia. In its Dept. of Genomics and Proteomics, crystallographic work is focused on the characterization of signal-transduction mechanisms (http://bit.ly/aqdxN6). V. Rubio (rubio@ibv.csic.es), head of the Structural Enzymopathology Unit, promoted the use of crystallography in this institute, A. Marina (amarina@ibv.csic.es) is the leader of the Crystallography of Macromolecules Unit, and J. Bravo (jbravo@ibv.csic.es) is the leader of the Signal Transduction Unit.

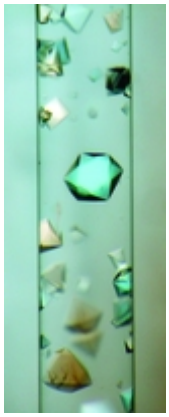
13. Andalusia

Andalusia, the second-largest Autonomous Community of Spain, occupies the south-east corner of the Iberian Peninsula. Andalusia was the center of power in medieval Muslim-dominated Iberia. Besides Muslim or 'Moorish' influences, the region's culture has been influenced by Iberians, Carthaginians, Greeks, Romans, Vandals and Visigoths, who preceded the Muslims, Castilian and other Christian North Iberian groups. Andalusia also had a relatively large Sephardic Jewish population. Many cultural characteristics that are internationally seen as 'typically Spanish' are largely of Andalusian origin.



A metal stabilized by CP's.

In Seville, the capital city, crystallographic activity is found in the Inst. of Material Science, a joint research centre between the U. of Seville and the CSIC, where M. J. Dianez (dianez@us.es), A. Justo (jjusto@icmse.csic.es), A. Criado (criado@us.es) and M. D. Estrada (estrada@us.es) provide crystallographic capabilities (http://bit.ly/bB9uHg). At the U. of Malaga, M. A. G. Aranda (g_aranda@uma.es) leads a group in the Dept. of Inorganic Chemistry, Crystallography and Mineralogy, working with inorganic solids with unusual conducting, magnetic or structural properties (http://bit.ly/afe1Ls).



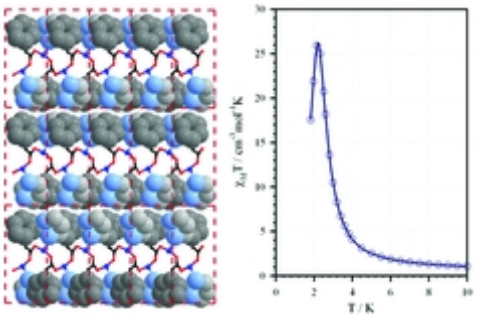
LEC: crystallization under diffusion-controlled mass transport.

Granada, the city of 'La Alhambra', located near to the highest peak in the Iberian Peninsula, Mulhacén (3,479 m), has two teams working in crystallography. At the U. of Granada, the crystallographic work done at the Coordination Chemistry and Structural Analysis group is led by D. Martín (jdmartin@ugr.es). The Laboratory for Crystallographic Studies (LEC), a joint Inst. of the CSIC and the U. of Granada, headed by J. M. García Ruiz (juanma.garciaruiz@gmail.com), is a group known for their expertise in nucleation and crystal growth, industrial crystallization, nonlinear systems and pattern formation, biomineralization and biomimetic materials. They are also known for their technological products, including the 'Granada crystallization box', an Advanced Protein Crystallization Facility, used in ESA's and NASA's spaceships. J. García Ruiz is the principal investigator of a joint project, The Spanish Factory of Crystallization (http://lafactoria.lec.csic.es/lafactoria/), formed by nine Spanish groups to create an integrated platform for research and services in crystallography. García Ruiz is also leading the 'Master and PhD in Crystallography and Crystallization' teaching program, a unique training opportunity for young investigators (http://lec.ugr.es/ and http://lafactoria.lec.csic.es/mcc).

Cadiz, the oldest continuously inhabited city in the Iberian Peninsula and possibly of all south-western Europe, has a general service diffraction unit headed by P. Valerga (pedro.valerga@uca.es).

At the U. of Almeria, A. Cámara (acamara@ual.es) leads a group of macromolecular crystallograpers in the Dept. of Physical Chemistry, Biochemistry and Inorganic Chemistry analysing polyproline recognition domains and their interaction with ligands (http://bit.ly/aMZDUJ).

14. Canary Islands



Metamagnetism in hydrophobically induced carboxylate(phenylmalonate)-bridged copper(II) layers.

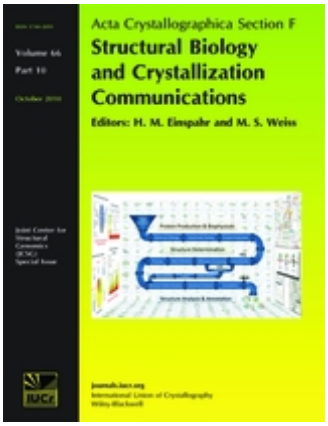
The Canary Islands are a Spanish archipelago of seven islands, located just off the northwest coast of mainland Africa, 100 km west of the border between Morocco and the Western Sahara. In the Dept. of Fundamental Physics II of the U. of La Laguna (Tenerife), powder and single-crystal services are provided by J. G. Platas (jplatas@ull.es), who also shares with C. G. Silgo (csilgo@ull.es) a crystallographic research team (http://bit.ly/dC1OEH). The Laboratory of X-ray and Molecular Materials, also at the U. of La Laguna, studies multi-functional magnetic molecular materials, seeks new applications for this type of materials, conducts synthesis of new ligands, coordination chemistry of selected carboxylates, systematic synthesis for crystal engineering and preparation of precursors for magnetism. The group leader is C. Ruíz-Pérez. Neutron and Synchrotron data complement X-ray diffraction techniques (caruiz@ull.es) (http://bit.ly/97zxMa).

We all kindly invite you to participate in IUCr2011.

Compiled by M. Martinez-Ripoll

IUCR ACTIVITIES

Acta Crystallographica Section F showcases structural genomics publications



The application of high-throughput methods to structural biology has generated an abundance of new macromolecular structures. In order to help ease the resultant publication backlog, *Acta Crystallographica Section F* now offers a special publication strategy to showcase these structures and the experiments upon which they are based. The first example was published in December 2009 and contained eight papers from the RIKEN-UK structural genomics consortium in a special section of the journal.

More recently (October 2010), the journal published a special issue that focuses exclusively on 35 structures, grouped into context, from the Protein Structure Initiative Joint Center for Structural Genomics. The issue, which is open access, is available from http://journals.iucr.org/f/issues/2010/10/00/issconts.html. This milestone publication has been enthusiastically welcomed by the community, and new requests and proposals for further special issues and special sections are under consideration.

For more information, please contact the Editors, Howard Einspahr (hmeinspahr@yahoo.com) or Manfred Weiss (msweiss@helmholtz-berlin.de).

MEETING REPORT

2009 Croatian-Slovenian Meeting

Varazdin, Croatia, June 2009

www.hazu.hr/kristalografi/varazdinmeeting/index.htm



The opening of the Meeting: Ivan Leban and Stanko Popovic.

The 18th Croatian-Slovenian Crystallographic Meeting featured 5 plenary lectures and 37 oral contributions, and was attended by 108 crystallographers from 14 countries. From Kari Rissanen (Jyvaskyla, Finland) we heard about exciting research in supramolecular chemistry from Pacman to intermolecular interactions. Sasa Petricek (Ljubljana, Slovenia) surveyed a broad range of polyether complexes. Pance Naumov (Osaka, Japan) summarized development in the field of solid-state photochemistry including ultrafast photodiffraction. Fred Antson (York, UK) opened for us an exciting world of bacteriophages, molecular motors and DNA translocation. Pavo Dubcek (Zagreb, Croatia) described small-angle scattering from thin films. In other presentations, the attendees learned many ways to combine X-ray diffraction with EPR, Raman, IR, NMR, mass spectroscpoy, electron microscopy and thermal analysis. We were told that simple disorder is bad enough but that triple and quadruple disorder is far worse. We also learned about kidney stones, egg white coagulation, the subtle distinction between binuclear and dimeric, that the Gingko tree is from the Jurassic period, certain organic compounds are stable at 800°C, water and Mg^{2+} are isoelectronic species, and there are no $N(phenyl)_4^+$ species. Furthermore, I found out that 'semiquinones' in the hotel prevented me from sleeping, I should drink more coffee, and that the colour 'green' is unusual for radical political parties.



Participants listening to the plenary lecture; Karl Fischer in the first row.

We want to express appreciation to all members of the organizing committee. A. Visnjevac and Z. Stefanic created a wonderful website for the Croatian Crystallographic Assn, and processed all abstracts and registration with assistance from M. Cetina. This Meeting would not have been possible at all without help of the sponsors Renacon (Zagreb), Panalytical, SCAN (Preddvor), JEOL, Dectris (Baden), Hecus (Graz), Incoatec (Geesthacht), Skolska Knjiga (Zagreb), Oxford Diffraction (Yarnton), Hotel Turist

(Varazdin), and the Ministry of Science, Education and Sport (Croatia). Further details describing the meeting and a photo album are available on the website.

Ivan Leban and Stanko Popovic, Meeting Co-chairmen

MEETING REPORT

CrSJ 2009 General Assembly

Hyogo, Japan, December 2009

http://sci-tech.ksc.kwansei.ac.jp/crsj2009/index-e.html



Left to right: A. Takenaka (President), K. Wada, Y. Ohashi, A. Nakagawa, K. Sugiyama and R. Kiyanagi.
The Annual Meeting and General Assembly of the Crystallographic Society of Japan was held at Kwansei Gakuin U., December 5-6, 2009. 33 years have passed since the last annual meeting was held in the same university. The meeting featured 3 symposia, 72 oral and 135 poster presentations covering all aspects of crystallography, and an industrial exhibition. 373 crystallographers attended the meeting.

The symposia were on 'Studies of new materials science using open X-ray free-electron lasers', 'Crystal chemistry using powder X-ray structure analysis' and 'Behavior of protein molecules seen from more advanced information of the crystal structure'. They were organized by J. Mizuki (JAEA), Y. Ozawa (Hyogo Pref. Univ.) and K. Miki (Kyoto U.), respectively.

The first symposium included lectures by K. Tohno (RIKEN Inst.), Y. Tanaka (RIKEN Harima Inst.), E. Matsubara (Kyoto U.) and H. Kakuta (Tohoku U.). The optical characteristics of the X-ray free-electron laser, its application to materials science, and new technologies were discussed.

The second symposium included lectures by M. Takaya (Kyoto U.), M. Kawano (POSTECH, AMS), Y. Kubota (Osaka Pref. U.), and H. Uekusa (Tokyo Inst. Tech.). Characteristic properties and powder X-ray structural analyses of molecules concerning supermolecular assembly, instantly synthesized molecules of coordination network, nanoporous metal-organic solids and medical compounds were discussed.

The third symposium included lectures by K. Miki (Kyoto U.), R. Kuroki (JAEA), E. Yamashita (Osaka U.) and I. Tanaka (Hokkaido U.). Behavior of electrons or hydrogen atoms in protein detected by super-high resolution analyses or by neutron diffraction were discussed. Behaviors of supermolecules detected by middle- or low-resolution X-ray data and a new approach for drug discovery by using the information of small molecules trapped in the crystal were also discussed.



Left to right: K. Ohsumi and Y. Ohashi.
At the Awards Ceremony, the S. Nishikawa Award was presented to Y. Ohashi (JAERI). Research Awards were given to A. Nakagawa (Osaka U.) and K. Sugiyama (Tohoku U.), and The Young Crystallographer

Awards went to K. Wada (Osaka U.) and R. Kiyanagi (Tohoku U.). At the general meeting, K. Ohsumi (Prof. Emer. KEK) and Y. Ohashi (Prof. Emer. Tokyo Inst. Tech.) became honorary members of our society. The Nishikawa memorial lecture and two award lectures were presented by Ohashi, Sugiyama and Nakagawa, respectively.

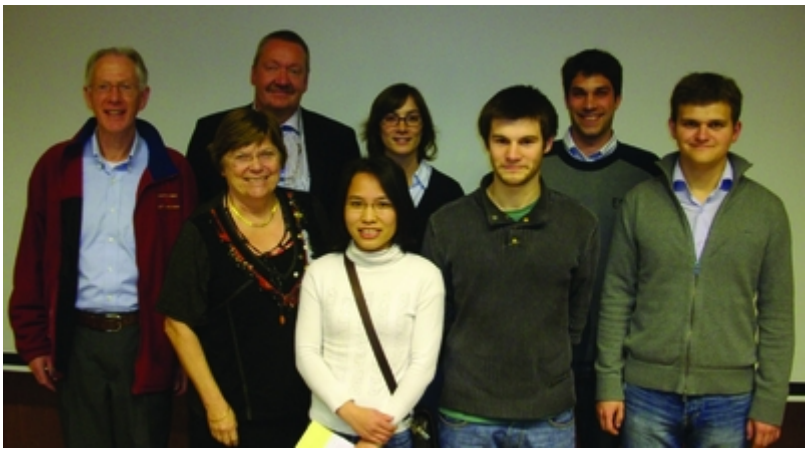
The local chair was H. Terauchi (Kwansei U.) and program chair was I. Takahashi (Kwansei U.). Details of the program can be viewed on the website.

Tsuyoshi Inoue

MEETING REPORT

Sixth Belgian Symposium

Brussels, Belgium, October 2010, www.chem.kuleuven.be/bcc/bcs/



Speakers and poster prize winners at the Sixth Belgian Crystallography Symposium BCS-6. From left to right: Martin Caffrey, Sine Larsen, Wim Bras, Ngan Bich Nguyen, Marta Saraiva, Mathieu Rocaboy, Maxime Baijot, Dmitry Batuk.

More than 100 scientists took part in the Sixth Belgian Crystallography Symposium BCS-6, held October 13, 2010, at the Academy House, adjacent to the Royal Palace in Brussels, under the aegis of the Belgian National Committee for Crystallography. Due to the success of previous BCS meetings, the National Committee for Crystallography organizes this symposium at biennial intervals to promote contacts between Belgian scientists using diffraction and microscopy techniques for studies in the fields of condensed matter chemistry and physics, material sciences, earth sciences and life sciences. As one of the main objectives was to promote personal contacts, plenary lectures were limited to three, given by distinguished colleagues in widely different fields. During the opening lecture by IUCr president, Sine Larsen, an overview of the activities and aims of the IUCr was given and directly related to the importance of large facilities for the advancement of the field of crystallography. Fullerenes and nanotubes are the favorite study materials of Paul Thiry (Namur), especially the helical 'Belgian' nanotubes discovered in Namur. The morning session was closed by Martin Caffrey (Dublin) with a talk on the promising approach of using lipidic mesophases in crystallizing membrane proteins. A poster session and commercial exhibition was organized during lunchtime. For the afternoon session, three oral presentations were selected from the submitted abstracts (Mathieu Rocaboy, Liège; Dmitry Batuk, Antwerp; and Marta Saraiva, Ghent). Poster prizes were awarded to Maxime Baijot (Liège) and Ngan Bich Nguyen (Leuven). On the occasion of its tenth anniversary, Wim Bras (Grenoble) highlighted the importance of the Dutch-Belgian beamline DUBBLE in Grenoble, currently resulting in more than 550 publications. The meeting was sponsored by the Royal Academies of Sciences and Art of Belgium, and by Bruker AXS, Oxford Diffraction, EFG Berlin, FEI Europe and JEOL.

Luc Van Meervelt

MEETING REPORT

The ECA Executive Committee's 'Winter Meeting' 2010

Budapest, Hungary, February 26-28, 2010

www.ecanews.org



The participants of the 'Winter Meeting' of the Executive Committee of the European Crystallographic Association, held February 2010 in Budapest, Hungary, at the Guest House of the Hungarian Academy of Sciences. From left to right: Massimo Nespolo (Education Coordinator and Webmaster), Radomír Kužel (Treasurer), Elena Boldyreva (IUCr Representative), Petra Bombicz (Secretary), Engin Kendi (ECM25), Hartmut Fuess (ECM26), Santiago García-Granda (President, in front), Andreas Roodt (Vice President, back), Wulf Depmeier (Officer), Süheyla Özbey (ECM25), John R. Helliwell (Past President), Alessia Bacchi (Officer) and Luc van Meervelt (Officer).

The Executive Committee (EC) of the European Crystallographic Association held its regular 'Winter Meeting' between 26th and 28th February 2010 in Budapest, Hungary. The ECA President, Santiago García-Granda, summarised the strategy of the Association using a risk and opportunities analysis covering the fields of ECA membership, scientific organisation, ECM organisation, professional development of ECA members, education and finances. Elena Boldyreva represented the IUCr. Wulf Depmeier of the EC overviewed the countries belonging to the ECA region. The focal points are encouraging the activity of Baltic countries, how to involve more countries in Africa and integration of new candidate countries into the Association. An important aim of the Association is to increase the number of individual members. Led by Luc van Meervelt, the bursary-funding applications of the organisers of schools, conferences and workshops were evaluated. The next application deadline is 1st February 2011.

The establishment of a 'General Interest Group - Network of Young Chemists' in the ECA region is in progress. Alessia Bacchi is organising this effort to support activities of the younger generation of crystallographers, such as their organisation of scientific meetings, sessions and exchange of information. By request, the parallel establishment of a General Interest Group for senior scientists is also proceeding. This GIG will work to preserve the history of crystallography, archive materials, play an important part in teaching, and consider the special requirements of senior scientists etc.

There is also an increasing effort focused on the education of future generations of crystallographers at all levels. As part of the process to establish a European Graduate School of Crystallography (Masters and PhD), Massimo Nespolo has submitted a proposal for an ERASMUS MUNDUS Master Course that will involve a collaboration of several universities, most importantly Université Henri Poincaré Nancy, Charles University Prague and Univerisità degli studi di Padova, with contributions from the universities of Antwerp, Liège, Pays Vasco, Aveiro and Oviedo, and the European Synchrotron Radiation Facility in Grenoble.

Alessia Bacchi is monitoring the performance of the SIGs. The aim is that all SIGs should have a website in the near future. The number of ECA individual members registered with each SIG does not reflect the total number of researchers involved in the work of the respective SIG. It is the task of the SIGs to convince as many researchers as possible to become ECA individual members and to express their explicit interest for the SIG's activities. There are several SIGs which coordinate or sponsor prizes or organize schools and workshops, in addition to participating in the work of the programme committees of the ECMs. They also organise keynote lectures and microsymposia. To strengthen contact with the SIGs, the ECA EC will continue its personal meetings with the SIG officers on the day of the opening ceremony of ECM meetings. Some SIGs already have a well established connection with the corresponding IUCr Commissions. The EC will encourage all the SIGs to form strong links with their corresponding IUCr Commissions.

The ECA Perutz and Bertaut Prize Committees, chaired by Andreas Root, work independently from the ECA EC. The Prizes will be awarded during ECM26 in Darmstadt. Donations to these Prizes' funds are possible via the ECM website.

The Organizers, Engin Kendi and Süheyla Özbey, of the very successful ECM25 Istanbul meeting gave a final report on the event. Hartmut Fuess, the next ECM26 Darmstadt chair, and Karl Törnroos, ECM27 Bergen, presented their organisation progress. Warwick University (UK) will host ECM28 to be held in 2013. For information on the European Crystallographic Association please visit the ECA News website: www.ecanews.org.

Petra Bombicz

OBITUARY

Eila Cedergren-Larsson (1937-2010)



Many chemists boast that they are great cooks, but few conduct research experiments at home in their kitchen. Eila Cedergren-Larsson combined the raising of three children with her scientific work and did the most crucial experiment of her PhD in her kitchen refrigerator. There she grew crystals of alcohol dehydrogenase that were visible to the eye and diffracted X-rays to atomic resolution. Her secret ingredient was an unconventional knack for getting the simple details right and a persistence that could break an elephant's back.

Eila Cedergen-Larsson of Lund University passed away in August 2010 as the result of a stroke. She was of Finnish descent and was evacuated to Sweden during World War II as a small child. After the war, she was returned to Finland where her family put her to work in a factory. She managed to convey her situation to her Swedish foster parents who came to her rescue and brought her back to Sweden. She often related this experience to young scientists from around the world to encourage them to persevere and follow their goals.

Eila had a life-long passion for her PhD project, alcohol dehydrogenase (ADH). In 1964 under the supervision of Carl-Ivar Branden in Uppsala, she studied different states of the enzyme and determined its structure in complex with different ligands. She probed distortions in ligand geometries and found that the then current paradigm for the textbook mechanism of ADH action was flawed. She worked on many other challenging projects, including dUTPases and their potential as drug targets against *Leishmania*, actin and bovine profilin. These were challenging proteins to work with due to their intrinsic polymerization properties. She was always interested in developing new technologies for crystallization, such as the little dialysis chambers she made in her kitchen, as well as a levitating droplet device.

Eila was always unconventional and adventurous and she had a gift for engaging young scientists through her contagious enthusiasm. She initiated a number of protein crystallization courses, such as the PEPC course at EMBL, that are still taught today. She would put the young guns at ease before a presentation by saying, 'All those important men? Just think of them in their underpants and they all become human.'

Rob Meijers

AWARDS AND PRIZES

Zbigniew Dauter receives highest science award from Polish Academy of Sciences



Zbigniew Dauter receives the Nicolaus Copernicus Medal from Michal Kleiber, President of the Polish Academy of Sciences. (Photo M. Mlekicki.)



On March 9, 2010, Michal Kleiber, President of the Polish Academy of Sciences, decorated Zbigniew Dauter with the Nicolaus Copernicus Medal, the highest distinction awarded by the Polish Academy of Sciences. The ceremony took place in the Staszic Palace in Warsaw. The award recognizes Dr. Dauter's contribution to the development of protein crystallographic methodology, in particular in the areas of phasing methods and macromolecular structure at ultimate resolution. His name is already permanently associated with the technique of quick halide soaks ('dauterization' of protein crystals), with the exploitation of weak anomalous signal (for example, of phosphorus in nucleic acid structures) and with the use of (jolly!) SAD phasing. He is an expert experimenter, widely known for his skills in getting the best possible diffraction data from macromolecular crystals. A graduate of the Gdansk U. of Technology, he obtained his PhD degree for crystallographic work on small-molecule drugs done with Zofia Kosturkiewicz (Poznan). His postdoctoral posts included work with Michael Woolfson (U. of York). Later Zbigniew (Zbyszek to friends) Dauter spent a number of years at several synchrotron centers (EMBL c/o DESY, Hamburg; NSLS, Brookhaven; APS, Argonne) conducting structural biological research and helping external users of macromolecular crystallography beamlines. The stations that he has supervised are among the most successful beamlines in protein crystallography. He has had a stunning number of collaborations, mostly because of his expertise in synchrotron data collection and structure determination. Currently, he is a principal investigator in the Macromolecular Crystallography Laboratory of the National Cancer Institute at Frederick, and facilitator for the NIH users of the SER-CAT beamline operating at the APS synchrotron in Argonne. The honor bestowed on Dr. Dauter will be felt in the wide circles of our crystallographic family. Congratulations, Zbyszek!

Mariusz Jaskolski