



INTERNATIONAL UNION OF Crystallography

NEWSLETTER

www.iucr.org

Volume 18, Number 3 ◆ 2010

CRYSTALLOGRAPHY IN SPAIN

The central graphic is a map of Spain overlaid with various 3D crystallographic models. In the northwest, a green metallic surface and a ball-and-stick model are shown. The north-central region features a pink polyhedral framework and a blue molecular model. The northeast shows a pink and blue ribbon representation of a protein. The south-central area includes a blue space-filling model and a yellow ribbon structure. The southwest has an orange space-filling model and a tan molecular model. The southern coast shows a colorful rainbow-like structure. The Balearic Islands are marked with small icons. An inset in the bottom right shows the Spanish flag and the IUCr logo.



A view of La Alhambra, Granada (XIII Century)

mensional space, which made the most important pre-Renaissance Spanish contribution to crystallography and geometrical art. The decorative symmetry of the tiling in the Alhambra Palace in Granada is today used to teach symmetry all over the world.

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



Sample of mosaics in La Alhambra (XIII Century).

ORGANIZED BY M. MARTINEZ-RIPOLL

Some historical and general outlines

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

The vast amount of mineralogical information contained in Pliny's "Natural History" was preserved and enhanced in "Book XVI on Stones and Metals" which covered the Etymologiarum of Isidor of Seville (560-636). It is also in the Lapidarium of Alfonso X (1221-1284), a fascinating work by a group of Muslim, Hebrew and Christian sages from a time when peaceful multicultural collaboration was demonstrated to be possible. Nevertheless, it was the unparalleled talent of the Arabian geometers in investigating the problem of tessellation of two-di-



A sample of Lapis specularis.



Deposits of Lapis specularis in Segóbriga.

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

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

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



Some crystallographic models of the abate Häuy

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



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

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

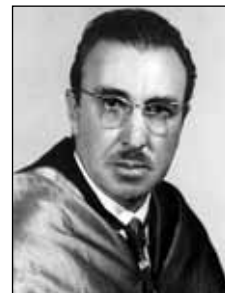


Blas Cabrera
(1878-1945)

Gabriel M. Cardoso
(1896-1954)

Julio Palacios
(1891-1970)

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



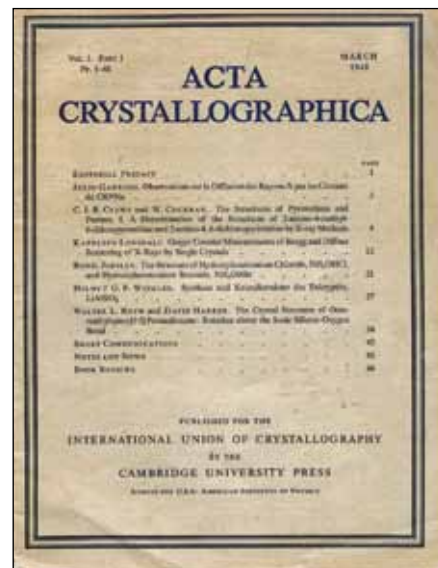
Luis Brú (1909-1997)

After the Spanish Civil War young crystallographers created the foundations of current Spanish crystallography, L. Bru advanced X-ray and electron microscopy first in the Canary Islands, later in Sevilla and finally at the U. of Madrid. L. Rivoir headed the X-ray Dept. at the Instituto de Física, Consejo Superior de Investigaciones Científicas (CSIC), the Spanish National Research Council and J. L. Amorós formed a group of young crystallographers and crystal growers at the U. of Madrid.



José L. Amorós (1920-2001) Julio Garrido Mareca (1911-1982)

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





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

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

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

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

The importance of crystallography for the development of chemistry in Spain led to the growth of several crystallographic groups. In this enterprise a generation of young Spanish crystallographers born around 1940 played an important role, elevating Spanish crystallography to its rightful place on the international stage. Many of them have passed away, including F.H. Cano (CSIC) and X. Solans (U. of Barcelona), others have retired such as J. Fayos and Francisco Sanz (CSIC), and J.A. Subirana (Polytechnic U. of Barcelona), while others are still active including Carlos Miravittles, C. Foces-Foces, E. Iglesias, M. Martínez-Ripoll (CSIC) and J.M. Amigó (U. of Valencia). However, crystallography in Spain, and especially in academic institutions, still seems to be erroneously considered a minor technical skill, whose application and interpretation is trivial. Despite the importance of crystallography for biology and biomedicine, and the rather large number of research groups in Spain in cellular

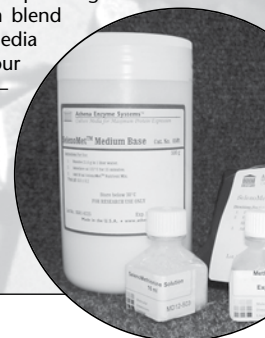
Optimize expression

Ready-to-use SelenoMethionine media – exclusive to Molecular Dimensions.

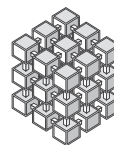
Based on a synthetic M9 minimal media supplemented with glucose, vitamins and amino acids with the exception of L-methionine.

A glucose-free option is available for testing with Novagen's Overnight Express™ Autoinduction System I.

Turbo™Broth, Superior™Broth, Hyper™Broth and Power™Broth are high performance media for expressing proteins in *E.coli*. To determine which blend works best for your protein, our Media Optimization Kit™ contains these four formulas and two standard media – enough to do 40 screens. Best of all the kit reduces expression optimization to just 1 day.



**Intelligent solutions
for protein crystal growth**

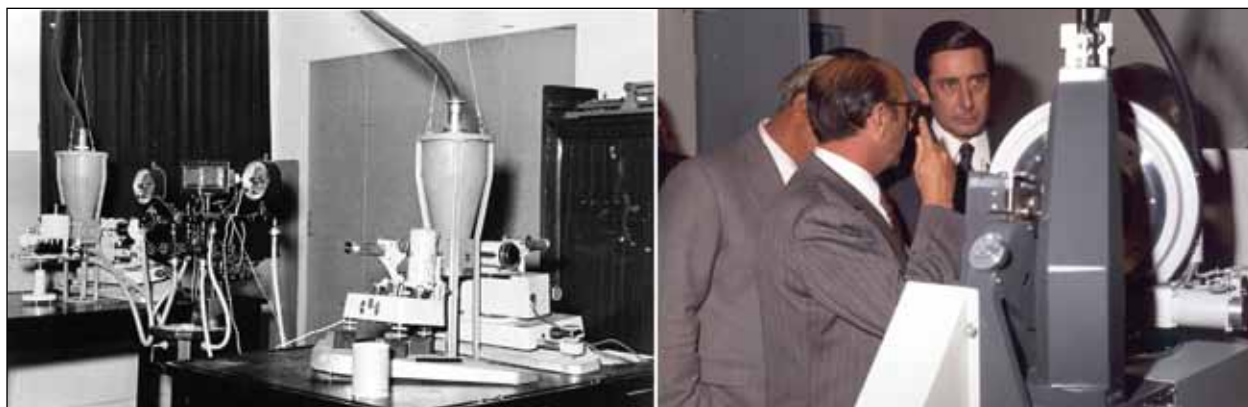


**Molecular
Dimensions**

moleculardimensions.com

and molecular biology, the lack of resources dedicated to macromolecular crystallography is very apparent. At the end of the eighties Spain became the first associate scientific member of the Institute Laue-Langevin (ILL), the high flux neutron reactor of Grenoble and new possibilities were opened for the crystallographic community including physicists, biologists, and engineers. Increased activity developed around magnetic crystallography, soft condensed matter, liquids and amorphous systems and biology. Synchrotron techniques for crystallographic studies brought Spanish crystallographers to the European Synchrotron Radiation Facility (ESRF).

Today the Spanish Group on Crystallography and Crystal Growth (Grupo Especializado de Cristalografía y Crecimiento Cristalino, GE3C) has over 200 members. If other crystallographers associated with neutron, solid state, proteomics, and surface appli-



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



View of the Spanish synchrotron ALBA as in November 2009

cations, are taken into account then about 400 Spanish researchers are currently involved in crystallographic research. Most Spanish crystallographers are organized in teams in the Canary Islands, Andalusia, Valencia, Asturias, Catalonia, Galicia, the Basque Country and Madrid, as well as others. They share over 200 X-ray diffraction machines for both powder and single crystals applications, and maintain active participation in neutron and synchrotron techniques in different European facilities (the ILL, and the ESRF). The Spanish synchrotron ALBA, was inaugurated in March 2010 with several crystallographic beam lines. Electron microscopy will also be well represented there, from high resolution transmission electron microscopy to field emission electron scanning microscopy.

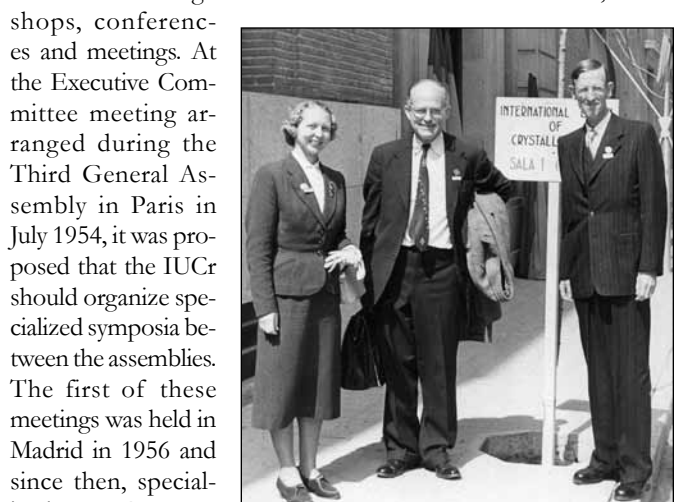


J.M. Bijvoet and his wife (Madrid, 1956)



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

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



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

Thanks to the explicit votes of Mario Nardelli (Italy) and Olga Kennard (UK), as well as to the financial support given by



Meeting on Anomalous Scattering, held in Madrid in 1974



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

M. Font-Altaba (the Mayor of Barcelona) the 6th European Crystallographic Meeting (ECM-6) was successfully held in Barcelona during the summer of 1980, with Carlos Miravittles as Chairman.

Now nearly one hundred years since the Laue and Bragg's experiments we are preparing to host the XXII Congress and General Assembly of the International Union of Crystallography (www.iucr2011madrid.es/) in Madrid. It will be a spectacular and memorable event from both scientific and social perspectives (see Page 23 for more on the Congress). ♦



Next Issue... "Crystallographers in Spain"

LETTERS TO THE EDITOR

Dear Judy and Bill,

With regard to Andrew Booth's recollections of his *Life in Science* part of the *Crystallography in Canada* article (V18, N2). I am curious why he misidentified Sam Levene as Aaron Klug, at the left in the back row of the photo of "The Bernal Team"? Booth must know that Klug did not arrive at Bernal's Lab until the end of 1953, to work with Harry Carlisle. Furthermore, why did he identify the photo as taken in 1948? The photo was taken in 1946 at the Royal Institution Faraday Lab, where Bernal's Birkbeck College crystallography group was temporarily housed immediately after the end of WWII. Booth correctly notes that he was away in the USA in 1946 (when the photo was taken), to attend the first ASXRED conference and to visit nascent US computer centers (a trip that Bernal had arranged for him). In 1946, Aaron Klug was starting work as a research student with R W James in Cape Town, South Africa and did not arrive in the UK until 1949 (at Cambridge). In 1948, Bernal and his "Team", including Andrew Booth, moved to the Birkbeck Crystallography Lab housed in a pair of near derelict terrace houses at 21, 22 Torrington Square, London. Rosalind Franklin moved there in March, 1953 and Klug began work with her there the following year. After her untimely death in 1958, Klug headed her group and, in 1962, moved with Ken Holmes and John Finch to the new MRC Laboratory of Molecular Biology in Cambridge, the same year that Booth moved to Saskatchewan.

DON CASPAR

rayonix
mx series

Seamless multi-element
CCD X-ray detectors



mx325/mx300

- 16 CCDs
- 4k × 4k readout in 1 sec.

mx225

- 9 CCDs
- 3k × 3k readout in 1 sec.

- Low noise
- Lowest achievable dark current
- Large area for protein crystallography

Options:

- Ultrastable baseline for SAXS/WAXS
- Custom taper ratios
- Custom phosphor options
- High resolution unbinned readout



High Efficiency models available

High electro-optical gain design



High Speed models available

10 to 100 frames/sec,
1 msec dead time

rayonix
SX165

Single CCD design

Options:

- Ultrastable baseline for SAXS/WAXS
- Custom taper ratios
- 4k × 4k resolution
- Custom phosphor options
- Frameshift option for time-resolved work



www.rayonix.com

1880 Oak Avenue Tel: +1 (847) 869-1548
Evanston, IL 60201 USA Fax: +1 (847) 869-1587
info@rayonix.com Toll Free in USA: (877) 627-XRAY

rayonix

High-performance X-ray technology