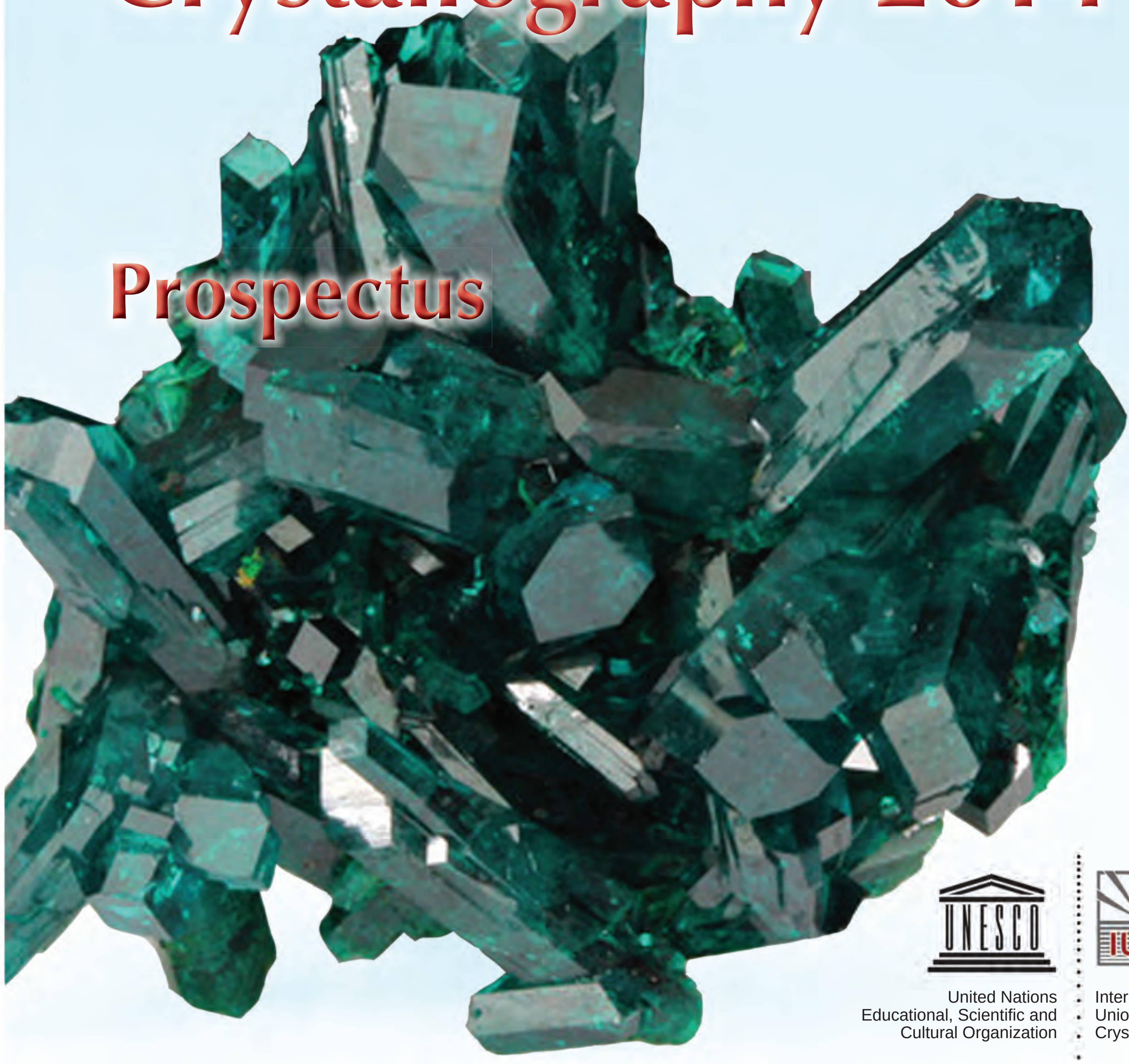
# International Year of Crystallography 2014

## Prospectus



United Nations Educational, Scientific and Cultural Organization

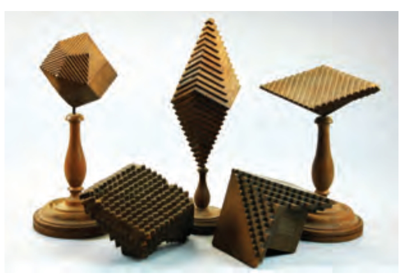
International Union of Crystallography

Partners for the International Year of Crystallography 2014

www.iycr2014.org

# International Year of Crystallography – 2014

Crystals – familiar to all in gemstones, glittering snowflakes or grains of salt – are everywhere in nature. The study of their inner structure and properties gives us our deepest insights into the arrangement of atoms in the solid state. From these insights has come the understanding needed to advance the sciences of chemistry, solid-state physics and, perhaps surprisingly, biology and medicine. A century has passed since crystals first yielded their secrets to X-rays. In that time, crystallography has become the very core of structural science, showing us the structure of DNA, allowing us to understand and fabricate computer memories, showing us how proteins are created in cells, and helping us to design powerful new materials and drugs. It also underpins investigations of cultural heritage artefacts. That is why in July 2012, following a proposal from Morocco, the General Assembly of the United Nations adopted the resolution that 2014 should be the International Year of Crystallography, 100 years since the award of the Nobel Prize for the discovery of X-ray diffraction by crystals.



# Goals

The International Year of Crystallography 2014 (IYCr2014) commemorates not only the centennial of X-ray diffraction, which allowed the detailed study of crystalline material, but also the 400th anniversary of Kepler's observation in 1611 of the symmetrical form of ice crystals, which began the wider study of the role of symmetry in matter. The major objectives of the IYCr2014 are:

- to increase public awareness of the science of crystallography and how it underpins most technological developments in our modern society
- to inspire young people through public exhibitions, conferences and hands-on demonstrations in schools
- to illustrate the universality of science
- to intensify the programme Crystallography in Africa and create similar programmes in Asia and Latin America
- to foster international collaboration between scientists worldwide, especially North–South contributions
- to promote education and research in crystallography and its links to other sciences
- to involve the large synchrotron and neutron radiation facilities worldwide in the celebrations of IYCr2014, including the SESAME project set up under UNESCO auspices

The lead sponsor of IYCr2014 is the International Union of Crystallography (IUCr) (www.iucr.org). The IUCr is an International Scientific Union founded in 1948, specifically to promote international cooperation among scientists and to promote the growth of the science of crystallography through research, publication and education.

The lead partner of IYCr2014 is UNESCO. For IYCr2014, UNESCO will act through its International Basic Services Programme (IBSP).

# Development of crystallography

Since the beginning of time, people have been fascinated by the beauty, purity, mystery and properties of crystals. Their regularity puzzled many philosophers, scholars and scientists, such as Pliny the Elder, who, 2000 years ago, in his *Naturalis Historia*, was fascinated by the "regularity of the six-sided prisms of rock crystals". The crystallization of salt and sugar was known to the ancient Indian and Chinese civilizations. Four centuries ago, Kepler (1611) tried to understand the formation of ice crystals in terms of compact packing of six units around a seventh one. 160 years later, Haüy showed that the shapes of crystals could be obtained by an appropriate three-dimensional packing of identical parallelepipeds that he called "molécules intégrantes". During the 19th century modern geometrical crystallography developed with formal mathematical descriptions of crystals based on symmetry (Hessel, Bravais, Sohnke, Fedorov, Barlow, Schönflies). A complete theoretical geometrical background had been developed by the time X-rays were discovered by Röntgen in 1895. A few years later, in 1912, Laue and his co-workers carried out a revolutionary experiment: they demonstrated how X-rays travelling into a crystal interact with it and are diffracted in particular directions depending on the nature of the crystal.

Laue's brilliant experiment marks the birth of radiocrystallography. A year later, father and son William Henry and William Lawrence Bragg related the directions and intensities of the diffracted beams to the atomic structure of the crystals. They showed that X-rays can be used to determine accurately the positions of atoms within a crystal and thus unravel its three-dimensional structure. This discovery has contributed hugely to the modern development of all the natural sciences, because atomic structure governs chemical and biological properties of matter, and the crystal structure determines most of its physical properties. Both Laue and the Braggs were honoured with Nobel Prizes (in 1914 and 1915).

Breakthroughs in the physical sciences followed in rapid succession. In chemistry, the determination of the crystal structure of hexamethylenetetramine by Dickinson and Raymond in 1923 definitively showed that molecules have a three-dimensional arrangement and exist discretely in a crystal, separated from each other by distances greater than the molecular covalent bonds. In biology, a fundamental advance occurred in 1953 with the discovery of the structure of DNA by Watson and Crick based on diffraction experiments performed by Rosalind Franklin. This ground-breaking discovery opened the door to macromolecular and protein

crystallography. There followed in quick succession the solution of the structures of other protein structures of profound biological importance: myoglobin, haemoglobin, insulin, vitamins – recognized by further Nobel Prizes, awarded in 1962 to Kendrew and Perutz, and in 1964 to Dorothy Hodgkin. Following these discoveries, the enthusiasm of scientists in many fields (mathematicians, physicists, chemists) for crystallography drove an extraordinary development of methodology, leading to the invention of the most important modern methods for solving crystal structures. The utmost importance of this work was recognized by another Nobel Prize to Hauptman and Karle in 1985.

The physical properties of crystals depend on their macroscopic symmetry and an accurate description of this allows the prediction of these properties. This was demonstrated in the birth of crystal optics 200 years ago and the exploration of fascinating properties such as birefringence. There followed the discovery of piezoelectricity by Pierre and Jacques Curie at the beginning of the 20th century; the first application of this was a sonar piezoelectric device developed in 1917 by Langevin.

As the main purpose of crystallography is to provide information on structure at the atomic or molecular scale, and as structure is intimately linked to the properties and functions of materials and molecules of all sizes, the impact of crystallography can be found everywhere in our daily world. Modern drug development, nano- and biotechnology are all based on crystallographic results. The properties of solid forms of active pharmaceutical ingredients depend heavily on their internal structure. Crystallographic experiments underpin the development of practically all new materials – from everyday materials like toothpaste, chocolate and computer memory, to advanced car and aerospace components – illustrating the strong ties between crystallography, industry and society. Indeed, crystallography permeates all structural science at the molecular level, including physics, biology, chemistry, mineralogy, geoscience and cultural heritage. Crystallography is thus an excellent example of the universality of science.

New sources for intense X-rays (synchrotrons, free-electron lasers) and neutrons that have been constructed during the last 20 years have revolutionized crystallographic science, and crystallography is the underlying science for all the experiments carried out at these large research facilities.

The crystallographic community has always had outstanding female practitioners (Dorothy Hodgkin was a 1964 Nobel Laureate). One of the 2009 Nobel Laureates was Ada Yonath, also a L'Oréal UNESCO Prize recipient in 2008. More recently, Irene Margiolaki, another crystallographer, was selected as L'Oréal UNESCO fellow 2010.

# Crystallography on the international stage

The growth of crystallography has always been associated with the organization of the crystallographic community. After 1918, 18 crystallographers from 6 countries decided to promote education and research in crystallography by writing the first version of the reference work now known as *International Tables for Crystallography* (1935), a definitive handbook of crystallographic knowledge and theory. Such collaborations contributed to the birth of the first crystallographic associations, ASXRED (the American Society for X-ray and Electron Diffraction, 1941) and XRAG (the UK X-ray Analysis Group, 1943). These came together at a meeting in the late 1940s where it was decided to form the IUCr and, uniquely for a scientific union, its own research journal *Acta Crystallographica*. The first Editor of this journal, in 1948, was P. P. Ewald, a student of Max von Laue. The first Conference and General Assembly of the IUCr was held in Harvard in 1948, with W. L. Bragg as the Union's first President.

Crystallographers worldwide are represented by the IUCr. The IUCr has been an active scientific union since its inception, promoting active research projects and standardization efforts through its many Commissions. It has also actively developed its publishing activities. The IUCr now publishes eight journal titles and eight volumes of *International Tables for Crystallography*. The IUCr's mission as a learned-society publisher is to serve the crystallographic community. The modest surplus of funds generated from its publishing activities is used to enable young scientists from less privileged countries to attend meetings and congresses worldwide and to stimulate international cooperation. Information on the activities of crystallographers worldwide is disseminated through the quarterly *IUCr Newsletter*. Over 10,000 scientists from 74 countries are registered with the IUCr's online directory of crystallographers. International Congresses, held every three years in different parts of the world, bring together close to 3000 scientists, at all stages of their careers, from the many different areas of crystallography. The IUCr's 20 scientific and two publishing Commissions are all international in composition. Regional Associates stimulate international cooperation in different geographical regions and play an important role in the promotion of crystallography in the North–South dialogue.

Knowledge of crystallography is a significant component for technological development and in the life sciences. One of the most important missions of the IUCr is to support education in crystallography in countries where the science is less developed. A successful programme entitled Crystallography in Africa is funded by the IUCr. This programme enables African colleagues to learn, practise and teach crystallography through basic and specialized schools. It also provides fellowships and bursaries for PhD students and young scientists to attend major crystallography meetings. It includes a significant collaboration with scientific instrument companies to ship free equipment to selected universities. An important objective of IYCr2014 is to extend such programmes to Asian and Latin-American countries.

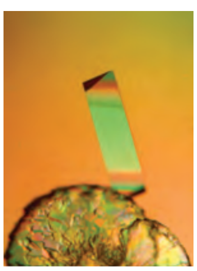
## International support for IYCr2014

The UN adopted the resolution that 2014 should be the International Year of Crystallography at its Sixty-Sixth General Assembly on 3 July 2012.

The lead sponsor (IUCr) and lead partner (UNESCO) are particularly grateful to Professor A. Thalal of the University Cadi Ayyad in Marrakech and the Moroccan Crystallographic Association who played a crucial role in preparing the resolution, which was most effectively presented by the permanent Moroccan UN delegation in New York.

Support for IYCr2014 has been received from the International Council for Science (ICSU) and its member scientific unions, including IUPAC (Pure and Applied Chemistry), IUPAB (Biophysics), IUPAP (Pure and Applied Physics), IUBMB (Biochemistry and Molecular Biology), IMU (Mathematics), IAU (Astronomy), IUHPS (History and Philosophy of Science), IUPHAR (Basic and Clinical Pharmacology) and IUFRO (Forest Research).

The active involvement of the 43 National Committees for Crystallography representing 52 countries, the National and Regional Crystallographic Associations and large-scale scientific facilities (SESAME for example) is welcome. Travelling exhibitions in Africa, the Middle East, Latin America and Asia will be based on scientific hubs in each region, and the willing involvement of these host centres reflects the widespread support for IYCr2014 and the importance of crystallography everywhere.



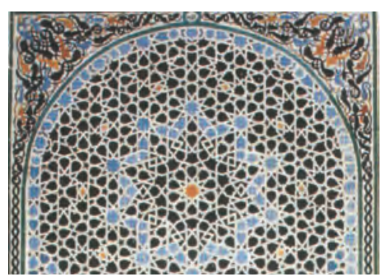
2014 international year of crystallography

## Activities and road map

In many of the larger countries, National Committees for Crystallography have already developed excellent educational materials that illustrate the impact of crystallography on society. IYCr2014 will be used by the IUCr and its Regional Associates as an opportunity to identify and organize these materials for broader use (with translation into major languages). A dedicated IYCr2014 web site has been established to disseminate these materials, and some will be developed into exhibits and demonstrations. This project will promote and create intense international collaborations.

IYCr2014 will have a strong educational component aimed at students of all ages. Countries that have experience in crystallographic education will organize and participate in training in countries that do not have a large crystallographic community. The IUCr has already arranged many successful workshops and schools to provide such training, and during IYCr2014 will organize schools in Africa, South America and Asia.

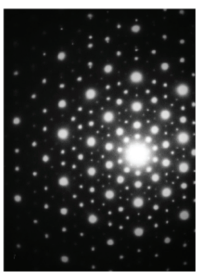
Travelling exhibitions for students will take place in Africa, the Middle East, Asia and Latin America in collaboration with diffractometer manufacturers. These exhibitions will have a hub in each region. From the hub, the exhibition will travel to selected universities with two or three instructors; for other universities, bursaries will be given for students to attend a regional exhibition at the hub. The exhibitions will comprise posters and lectures or workshops, along with hands-on experiments including the use of mobile diffractometers. The exhibitions will also be associated with a subsequent fellowship after 2014. This activity will increase global awareness of crystallography and, in the longer term, will have an impact on international collaborations and the worldwide development of science-based technologies.



The 43 Adhering Bodies of the IUCr, representing 52 countries, and its three Regional Associates have been invited to generate ideas for appropriate activities. Proposals will be listed on the IYCr2014 website.

Activities will include:

- Organizing travelling hands-on exhibitions
- Launching an open-access crystallography journal
- Providing all levels of students, from pre-school to university, with crystallography demonstrations at appropriate levels
- Publicizing the contributions that crystallographers make to the global economy by submitting articles to the press and to magazines or developing television and radio programmes
- Sponsoring poster exhibitions highlighting the usefulness and wonders of crystallography
- Organizing problem-solving projects through which students can use their knowledge of crystallography, physics and chemistry
- Publicizing the contributions that crystallography has made to improve lives, particularly recent developments in drug design and material science
- Organizing crystal-growing competitions
- Interacting with governments to underscore the importance of a strong crystallographic education
- Organizing consultations concerning the best ways to save all diffraction data collected in large-scale facilities and crystallography laboratories



A “toolkit” of ideas for organizers of IYCr2014 events will be made available. The IYCr2014 web site will include links to national crystallography celebrations worldwide and list IYCr2014 activities.

## Timetable

### Before December 2012

- Preliminary meetings with UNESCO representatives to define initial collaborations
- IYCr2014 committee determines actions to be carried out and the ways to realize them
- IYCr2014 logo designed via an open competition and launched during the IUCr Madrid Congress in August 2011
- Communication with National Committees and Regional Associates
- Web site version 1 launched
- Münich Laue conference

### December 2012

- AsCA 12/CRYSTAL 28 Adelaide conference and special Bragg symposium
- Fundraising begins
- Project Manager for IYCr2014 hired
- Large-scale facilities, crystallographic databases and other crystallographic organizations contacted

### January 2013–December 2013

- Web site version 2 launched
- Production of a booklet in electronic format for high-school students
- Preparation of Opening and Closing Ceremonies
- Fundraising
- Selection of the projects to be sponsored
- Work with the local hubs and diffractometer manufacturers to prepare the travelling exhibitions
- Preparation of crystallographic books and educational material
- Collaboration with scientific unions, TWAS and other scientific associations

### 2014: Implementation

- Opening Ceremony (Paris, France)
- Global events
- Travelling exhibitions
- Regional and national events
- IUCr Congress, Montreal, August 2014
- Closing Ceremony (Marrakech, Morocco)

### 2015

- Evaluation and follow up
- Final report
- Fundraising for follow up

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UNESCO contributes to the building of peace, the alleviation of poverty, sustainable development and intercultural dialogue through education, science, culture and communication. In fulfilling its mission, UNESCO functions as a laboratory of ideas and a standard-setter to forge universal agreements on emerging ethical issues. The Organization also serves as a clearinghouse – for the dissemination and sharing of information and knowledge – while helping Member States to build their human and institutional capacities in diverse fields. Through these activities, UNESCO promotes international cooperation among its 193 Member States and six Associate Members. Its programmes in natural sciences focus on mobilizing science knowledge and policy for sustainable development in the areas of basic sciences, science education, ecological and earth sciences, water sciences and climate change. More information about UNESCO and its activities in the natural sciences is available at www.unesco.org/science.

The IUCr is an International Scientific Union and a member of ICSU. Its objectives are to promote international cooperation in crystallography and to contribute to all aspects of crystallography, to promote international publication of crystallographic research, to facilitate standardization of methods, units, nomenclatures and symbols, and to form a focus for the relations of crystallography to other sciences.

## Contacts

G.R. Desiraju
IUCr President
Tel.: +91 80 22933311
E-mail: desiraju@sscu.iisc.ernet.in

C. Lecomte
IUCr Vice-President
Tel.: (33 0) 383684865
E-mail: claude.lecomte@crm2.uhp-nancy.fr

A. Thalal
Department of Physics, Faculty of Sciences
University Cadi Ayyad, Semlalia
Bd du Prince My Abdellah, Marrakech 40000, Morocco
Tel.: 212 (0) 6 63 21 10 18
E-mail: thalal@uca.ma

M.H. Dacombe
IUCr Executive Secretary
2 Abbey Square, Chester CH1 2HU, UK
Tel.: +44 1244 345431
E-mail: execsec@iucr.org

M. Nalecz
Director, Executive Secretary
International Basic Sciences Programme
Secretary, SESAME Council
UNESCO HQ, Paris, France
Tel.: (33 1) 45683930
E-mail: m.nalecz@unesco.org

J. J.-P. Ngome Abiaga
International Basic Sciences Programme
UNESCO HQ, Paris, France
Tel.: (33 1) 53693224
E-mail: jj.ngome-abiaga@unesco.org

M. Zema
Project Manager for IYCr2014
5 Abbey Square, Chester CH1 2HU, UK
Tel.: +44 1244 342878
E-mail: iycr2014@iucr.org
WWW: www.iycr2014.org

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