



United Nations
Educational, Scientific and
Cultural Organization



International
Union of
Crystallography

Ah! Crystallography!

I, You See Crystals!



**24th Congress and General Assembly of the
International Union of Crystallography
21-28 August 2017, Hyderabad, India**



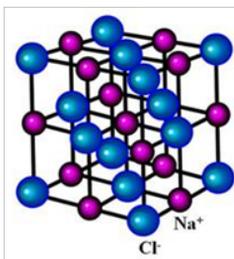
Adapted from a publication from UNESCO in 2014
for the 24th IUCr Congress in Hyderabad to be held in 2017



Printed in India



What is crystallography?



Common salt is a crystal. Its cubic symmetry results from the way in which sodium and chloride ions are bound to each other.

Crystals can be found everywhere in nature. They are particularly abundant in rock formations as minerals (gemstones, graphite) but can also be found elsewhere, examples being sugar, ice and grains of salt. Since ancient times, scholars have been intrigued by the beauty of crystals, their symmetrical shape and a variety of colours.

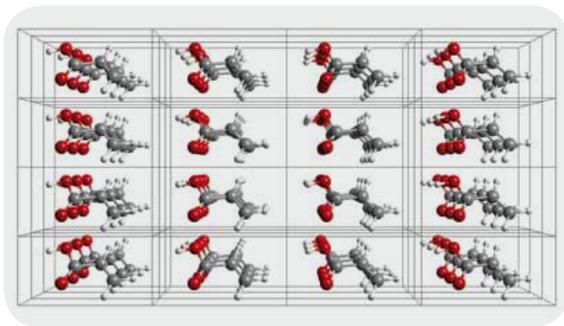
Early crystallographers used geometry to study the shape of crystals in the natural world. In the early 20th century, it was realized that X-rays could be used to 'see' the structure of matter. This marks the dawn of modern crystallography.

X-rays had been discovered in 1895. They are beams of light that are not visible to the human eye. When X-rays hit an object, the object's atoms scatter the beams. Crystallographers discovered that, in the case of crystals, their regular arrangement of atoms scattered the rays in just a few specific directions.

Ancient Indian writings refer to diamonds as the weapons of Indra, the warrior god. Valued at the time both for its exceptional hardness and the flashes of light given off by its natural crystal structure, the ancient Indian word for diamond was similar to the word thunder and lightning. Writings from the third century BC refer to the "octahedron crystal structure" of diamond and there is evidence that the ancient Indians used diamond tipped drills as early as the fourth century BC. Diamond is one of the simplest and internally most symmetrical of crystal structures. Many famous diamonds such as the Hope Diamond and the Koh-i-Noor Diamond were mined in Golconda in the Deccan, and the Koh-i-Noor was part of the Peacock Throne of Emperor Jehangir. The Jacob Diamond was a part of the jewellery collection of the Nizam of Hyderabad.



Koh-i-Noor Diamond



3D image of a crystal structure. In a crystal, atoms, groups of atoms, ions or molecules have a regular arrangement in three dimensions.

©Image: Michele Zema/IUCr

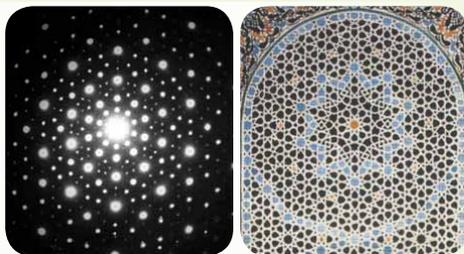
After 100 years of development, X-ray crystallography has become the leading technique for studying the atomic structure and related properties of materials. It is now at the centre of advances in many fields of science.

The development of machines capable of generating intense light and X-rays (synchrotrons) has revolutionized crystallography. X-rays (synchrotrons, free electron lasers) are used by crystallographers working in areas such as **biology, chemistry, materials science, physics, archaeology** and **geology**.

- Synchrotrons enable archaeologists to identify the composition and age, for example the composition and age of meteorites and lunar rocks.

QUASICRYSTALS: DEFYING THE LAWS OF NATURE?

In 1984, Dan Shechtman (Israel) discovered the existence of a crystal in which the atoms were assembled in a model that could not be strictly repeated. This defied the accepted wisdom about the symmetry of crystals. Up until then, it had been thought that only geometric forms with 1, 2, 3, 4 or 6 sides could occur as crystals, since only these forms could be reproduced in three dimensions. Yet, when Dan Shechtman observed an alloy of aluminium and manganese under an electron microscope, he discovered a pentagon (five-sided shape). This 'outlaw' came to be known as a quasicrystal. Dan Shechtman's groundbreaking discovery would earn him the Nobel Prize in Chemistry in 2011. Moroccan artisans (Maalems) have actually known about the patterns found in quasicrystals for centuries. Seven hundred years separate the two images below. The image on the left shows the diffraction pattern of a quasicrystal obtained by Dan Shechtman in 1984. The photo on the right shows a fine mosaic (zellij) in the Attaraine Madrasa in Fez (Morocco), dating from the 14th century. The images look remarkably similar, with both showing pentagonal patterns.



Source: diffraction pattern image, *Physical Review Letters* (1984), vol. 53, pages 1951–1953; mosaic, Moroccan Crystallographic Association

A brief history

Throughout history, people have been fascinated by the beauty and mystery of crystals. Two thousand years ago, Roman naturalist Pliny the Elder admired 'the regularity of the six-sided prisms of rock crystals.' At the time, the process of crystallizing sugar and salt was already known to the ancient Indian and Chinese civilizations: cane sugar crystals were manufactured from sugar cane juice in India and, in China, brine was boiled down into pure salt. Crystallization was also developed in Iraq in the 8th century CE. Two hundred years later, Egypt and the region of Andalusia in Spain would master the technique of cutting rock crystals for use in utensils and decorative items like the gem-studded box pictured here, which was made in Egypt in about 1200 CE. In 1611, German mathematician and astronomer Johannes Kepler was the first to observe the symmetrical shape of snowflakes and infer from their underlying structure.



IMPORTANT YEARS FOR CRYSTALLOGRAPHY:

1895: X-rays were discovered by William Conrad Röntgen, who was awarded the first Nobel Prize in Physics in 1901.

1914: Max von Laue and his co-workers discovered that X-rays travelling through a crystal interacted with it and, as a result, were diffracted in particular directions, depending on the nature of the crystal. This discovery earned von Laue the Nobel Prize in Physics.

1913: Father and son team William Henry Bragg and William Lawrence Bragg discovered that X-rays could be used to determine the positions of atoms within a crystal accurately and understand its three-dimensional structure. Known as Bragg's Law, this discovery has largely contributed to the modern development of all the natural sciences because the atomic structure governs the chemical and biological properties of matter and the crystal structure most physical properties of matter.

1915: William Henry Bragg and William Lawrence Bragg awarded Nobel prize in Physics

1920-1960s: X-ray crystallography helped to reveal some of the mysteries of biological structures. One of the biggest milestones of the 20th century was the determination of the crystal structure of DNA by James Watson and Francis Crick.

Dorothy Hodgkin, solved the structures of a number of biological molecules, including cholesterol (1937), vitamin B12 (1945), penicillin (1954) and insulin (1969). X-Ray methods provided answers that more traditional chemical methods could not provide. She was awarded a Nobel Prize in Chemistry in 1964

Crystallography and crystallographic methods have continued to develop over the last 50 years; in 1985, for example, the Nobel Prize in Chemistry was awarded to Herb Hauptman and Jerome Karle for developing new methods of analysing crystal structures.

Why we need to invest in crystallography

Crystallography supports the development of practically all new materials, from everyday products like computer memory cards to flat television screens, cars, aeroplane components and liquid crystals in many display devices. Crystallographers not only study the structure of materials but can also use this knowledge to modify a structure to give it new properties or to make it behave differently. The crystallographer can also establish the new material's 'fingerprint'. A company can then use this 'fingerprint' to prove that the new substance is unique when applying for a patent.

In fact, crystallography has many applications. It touches our daily lives and forms the backbone of industries which are increasingly dependent on knowledge generation to develop new products, including the agro-food, aeronautic, automobile, beauty care, computer, electro-mechanical, pharmaceutical and mining industries. Following are some of the examples.

Mineralogy is arguably the oldest branch of crystallography. X-ray crystallography has been the main method of determining the atomic structure of minerals and metals since the 1920s. Virtually everything we know about rocks, geological formations and the history of the Earth is based on crystallography. Even our knowledge of 'cosmic visitors' like meteorites comes from crystallography. This knowledge is generally essential for mining and any industry which drills into the Earth, such as the water, oil, gas and geothermal industries.

Drug design strongly depends on the use of crystallography. A pharmaceutical company looking for a new drug to combat a specific bacteria or virus first needs to find a small molecule capable of blocking the active proteins (enzymes) that are involved in attacking the human cell. Knowing the precise shape of the protein allows scientists to design drug compounds that can stick onto the 'active' sites on the protein and thereby disable their harmful activity.

Tip: Proteins are large biological molecules consisting of one or more chains of amino acids

Crystallography is also essential at the stage of drug manufacture. It is used in quality control of the processed drug during mass production, to ensure that strict health and safety guidelines are met.



Cocoa butter, the most important ingredient of chocolate, crystallizes in six different forms but only one melts pleasantly in the mouth and has the surface sheen and crisp hardness that make it so tasty. This 'tasty' crystal form is not very stable, however, so it tends to convert into the more stable form, which is dull, has a soft texture and melts only slowly in the mouth, producing a coarse and sandy sensation on the tongue. Luckily, the conversion is slow but if chocolate is stored for a long time or at a warm temperature, it can develop a 'bloom,' a white, filmy residue that results from recrystallization. Chocolate-makers thus have to use a sophisticated crystallization process to obtain the most desirable crystal form, the only one accepted by both gourmets and consumers.

The Curiosity rover used X-ray crystallography in October 2012 to analyse soil samples on the planet Mars! NASA had equipped the rover with a diffractometer. The results suggested that the Martian soil sample was similar to the weathered basaltic soils of Hawaiian volcanoes. Photo: NASA



Who organized the International Year of Crystallography?

The Year was organized jointly by the International Union of Crystallography (IUCr) and UNESCO.

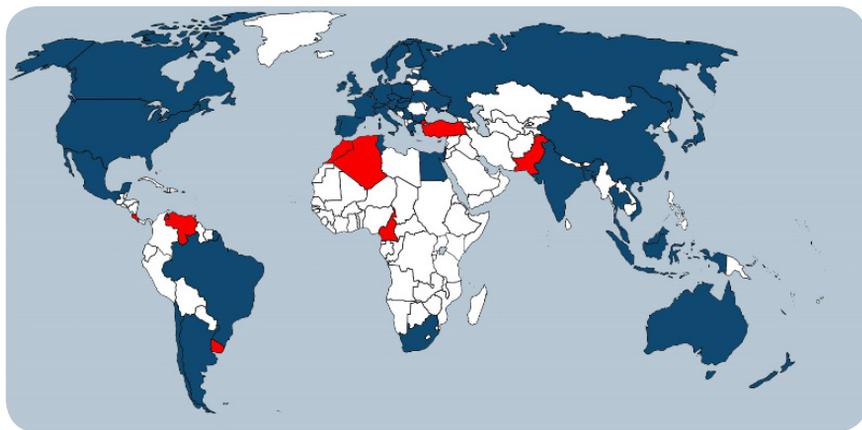
Aim...

- Even though crystallography connects all the sciences today, it remains relatively unknown to the general public. One aim of the Year was to promote education and public awareness through a variety of activities (see Who will benefit from the International Year of Crystallography?).
- There is a need to broaden the base of crystallography, in order to give more developing countries expertise in this critical field for their scientific and industrial development. This is all the more urgent in that crystallography will play a key role in the transition to sustainable development in coming decades.

Crystallographers are active in more than 80 countries, 53 of which are members of the International Union of Crystallography (IUCr). The IUCr ensures equal access to information and data for all its members and promotes international cooperation.

Countries that adhered to the IUCr before 2014 are shown in blue

Countries that joined in 2014 during IYCr are shown in red.



Challenges for the future

In 2000, the world's governments adopted the United Nations' Millennium Development Goals, which set specific targets to 2015 for reducing extreme poverty and hunger, improving access to clean water and safe sanitation, curbing child mortality and improving maternal health, among other challenges. Governments are presently preparing a fresh set of goals that will determine the development agenda for the post-2015 period.

The following are some examples of how crystallography can help to advance this agenda.

Food challenges

- Crystallography can be used to analyse soils, for instance. One serious cause of deteriorating soils is salinization, which can occur naturally or be induced by human activities.
- Structural studies on plant proteins can help develop crops which are more resistant to salty environments.
- Crystallography can also contribute to the development of cures for plant and animal diseases, one example being research into canker in crop species like tomatoes, or the development of vaccines to prevent diseases such as avian or swine flu.
- In addition, crystallographic studies of bacteria are important for the production of food products derived from milk, meat, vegetables and other plants.

Crystallography can identify new materials which can purify water for months at a time, such as nanosponges (tap filters) and nanotablets.
© Shutterstock/S_E

Water challenges

- Crystallography can help to improve water quality in poor communities, for instance, by identifying new materials which can purify water for months at a time, such as nanosponges (tap filters) and nanotablets.

Energy challenges

- Crystallography can develop new products which lower a home's energy consumption (and cooling bill) while curtailing carbon emissions, such as insulating materials. It can also identify new materials which reduce the cost of solar panels, windmills and batteries while making them more efficient, to reduce wastage and improve access to these green technologies.



Greening the chemical industry

- Crystallography can contribute to the development of ecological construction materials in developed and developing countries.
- It can also help to reduce pollution by replacing chemical solvents with 'green' inorganic solvents based on ionic liquids and CO₂.
- It can help to reduce mining waste and related costs by contributing to methods which selectively extract only the materials required.

Health challenges

- Crystallography can tackle the growing resistance of bacteria to antibiotics, for instance. Together with Venkatraman Ramakrishnan and Thomas Steitz, crystallographer Ada Yonath managed to determine the structure of the ribosome and the way it is disrupted by antibiotics. Ribosomes are responsible for the production of all proteins in living cells, including those of humans, plants and bacteria. If the work of the ribosome is impeded, the cell dies. Ribosomes are a key target for antibiotics, as antibiotics are able to attack the ribosomal activity of harmful bacteria while leaving human ribosomes untouched. In 2008, Prof. Yonath was awarded the L'Oréal-UNESCO Prize for Women in Science for her work and, a year later, all three scientists received the Nobel Prize.
- Crystallography can help countries to identify the properties and behavior of endogenous plants, with a view to developing skin and health care products, herbal remedies and so on.

Who will benefit from the International Year of Crystallography?

The Year targeted governments

By interacting with them and advising on the design of policies which:

- Finance the establishment and operation of at least one national crystallography centre per country;
- Develop cooperation with crystallography centres abroad, as well as with synchrotron and other large-scale facilities;
- Encourage the use of crystallography in research and development;
- Support research in crystallography;
- Introduce crystallography into school and university curricula, or modernize existing curricula.

The Year targeted schools and universities

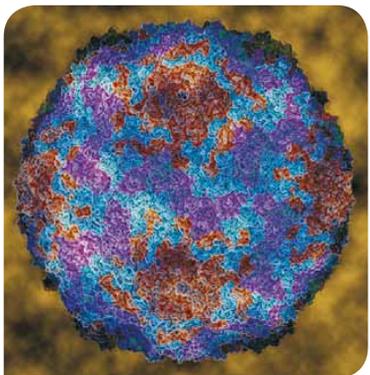
To introduce the teaching of crystallography where it is still absent, via, inter alia:

- Open laboratories prepared by the International Union of Crystallography which demonstrated how diffractometers work in countries in Asia, Africa and Latin America, in collaboration with diffractometer manufacturers;
- The ongoing Initiative in Africa for universities (see box) which was intensified and extended to countries in Asia and Latin America which lack crystallography teaching;
- Hands-on demonstrations and competitions in primary and secondary schools;
- Problem-solving projects for school pupils which use their knowledge of crystallography, physics, chemistry and biology

In the past 20 years, the number of people with diabetes worldwide has risen from 30 million to 230 million, according to the International Diabetes Federation. Had the structure of natural insulin, produced by the pancreas, not been determined by X-ray crystallography, it would be impossible to manufacture the life-saving biosynthetic 'human' insulin today.

Photo: Wikipedia Commons





Virus. You cannot design a drug without knowing the structure of relevant protein

The Year targeted the general public

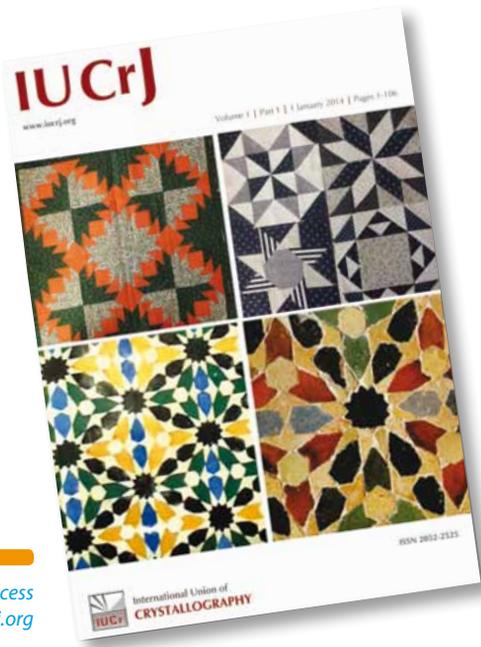
To increase awareness of the way in which crystallography underpins most of the technological developments in modern society but also its role in cultural heritage and art history, via:

- Public conferences organized by members of the International Union of Crystallography on themes like the paramount importance of protein crystal structures in drug design, crystallography and symmetry in art, or crystallographic analysis of artworks and ancient materials
- Sponsorship of poster exhibitions highlighting the usefulness and marvels of crystallography
- The submission of articles to the press, television and other media on the contribution crystallography makes to the global economy

The Year targeted the scientific community

To foster international collaboration between scientists worldwide, with an emphasis on North–South collaboration, via:

- The launch of an open access journal on crystallography (pictured), which is called IUCrJ. The first impact factor of IUCrJ is 3.105
- Joint research projects involving large synchrotron facilities in both developed and developing countries, such as the facility in Brazil or the SESAME facility in the Middle East born of a UNESCO project.
- Consultations to identify the best way to save all diffraction data collected in large-scale facilities and crystallography laboratories.



Copy of the first issue of open access journal available at www.iucrj.org

SYMMETRY IN ART AND ARCHITECTURE



Chinese symbol for happiness, pronounced shuangxi
Photo: Wikipedia



Taj Mahal, India, completed in 1648, today a UNESCO World Heritage property
Photo: Muhammad Mahdi Karim/Wiki Commons



Mayan temple in Chichen Itza in Mexico, which flourished from about 600 to 900 CE, today a UNESCO World Heritage property
©S. Schneegans/UNESCO

Be it a human face, a flower, a fish, a butterfly – or a non-living object like a seashell, symmetry pervades the natural world. It has always fascinated human civilizations, which have reflected symmetry in their art and architecture for thousands of years.

Symmetry can be found in all human expressions of creativity: carpets and rugs, pottery, ceramics, drawing, painting, poetry, sculpture, architecture, calligraphy. There is symmetry in the Chinese alphabet, for instance.

Art and architecture may demonstrate different forms of symmetry. A pattern that repeats itself indefinitely is said to show translational symmetry. It can be one-dimensional like a frieze, or two-dimensional like the winged animals in the image here.

In bilateral symmetry, the left and right sides are mirror images of one another. One example in nature is a butterfly. Bilateral symmetry has always been a common



Yoruba bronze head from the Nigerian city of Ife, 12th century CE
Photo: Wikipedia



Two-dimensional image by Maurits Cornelis Escher (Netherlands)
©MCEscher Foundation



Kolums like this one in Tamil Nadu are drawn in rice powder or chalk in front of homes to bring prosperity. They can be renewed daily.



Dome-shaped ceiling of the Lotfollah Mosque in Iran, completed in 1618, today a UNESCO World Heritage property ©Phillip Maiwald/Wikipedia

feature of architecture, historic examples being the Taj Mahal in India (pictured), the Forbidden City in China or the Mayan temple of Chichen Itza in Mexico (pictured). Bilateral symmetry is also common in art, although perfect symmetry in painting is rare. If a figure can be rotated about its axis or a particular point without changing the way it looked originally, it is said to show rotational symmetry. The pyramids of Giza in Egypt, for instance, show rotational symmetry of order four (including the base). The interior of the dome of the Lotfollah Mosque in Iran (pictured) shows rotational symmetry of order 32, starting around the point located at the centre of the figure.

Geometric patterns have pervaded the art of many civilizations. Examples are the sand paintings of the Navajo Indians, the kolam of south India (pictured), Indonesian batik (tie-dyeing), the art of Australian Aborigines, Tibetan mandalas and Hindu Srichakra (pictured).



Five Deity Mandala from Tibet, 17th century CE; mandala paintings always have a circle at their centre (mandala means circle in Sanskrit). Mandalas have spiritual significance in the Hindu and Buddhist religions. Source: Wikipedia Commons



The point, the triangle, the eight cornered figure, the ten edged figure, the 14 cornered figure, eight petals, 16 petals, the three circles, three squares, this is called Srichakra of the Supreme Deity in Hinduism



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Plenary Lectures

- **Susumu Kitagawa** - Crystallography of dynamic structures and properties of porous coordination polymers / metal - organic frameworks
- **John Spence** - Crystallography with X-ray lasers
- **Giacomo Chiari** - Crystallography in art and cultural heritage

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IUCr2017 Keynote Lectures

Name	Session Title
Simon J. L. Billinge	Application of PDF analysis to X-ray powder diffraction data
Vladislav Blatov	Topological approach for the design of new materials
Dario Braga	Making crystals with a purpose
David Bryce	Structure and properties of materials by solid-state nuclear magnetic resonance (SSNMR) observables
Jean Marc Castera	Traditional geometric patterns in India, and their specificities compared to Persian and Moroccan styles
Neil Champness	Two dimensional crystal engineering
Henry Chapman	Algorithms & instrumentation methods for 3D imaging with FEL pulses
Jon Eggert	Progress in high-pressure methodology and applications
Song Gao	Magnetic and electric anisotropy in molecular crystals
Juri Grin	Materials for energy
Michael Groll	Two decades of proteasome research: from structure to application
John Helliwell	The science is in the data
Richard Henderson	From electron crystallography to single particle CryoEM (Gjønnes medal lecture)
Jurg Hulliger	Combinatorial and solid state chemistry of polar molecular crystals
Dmitry Khalyavin	Magnetic degrees of freedom in emerging materials
Matteo Leoni	Microstructure, defects, stress and strain determination and modelling with powder diffraction data
Ron Lifshitz	Soft quasicrystals
Hartmut Luecke	Proton gated urea channel
Wladek Minor	Crystallographic tools towards understanding of macromolecular structure-function relationships
Ashwini Nangia	Pharmaceutical solids in crystal engineering
Massimo Nespolo	Crystallographic rationale for the formation of twinned crystals
Sakura Pascarelli	Science at high pressure: Evolution of magnetic and electronic properties and local structure in condensed matter

Vanessa Peterson	In situ and operando neutron and X-ray studies of functional materials
Ingrid J. Pickering	Synchrotron studies of metals in biological systems
Giuseppe Resnati	The halogen bond in crystal chemistry
Robin Rogers	Crystal engineering with ionic liquids
Bernhard Rupp	Validation of protein ligand structures
Leonid Sazanov	Respiratory complex I
Adriana Serquis	Crystallography of materials
Toshiyuki Shimizu	Structural biology of toll-like receptors
Janet Smith	Biological functions at the molecular level through multiwavelength anomalous diffraction
Dietmar Stalke	Application of charge density to organic and organometallic chemistry
Sriram Subramaniam	Insight into atomic structure of macromolecules by CryoEM
Dmitri Svergun	Small-angle x-ray scattering for biological macromolecules
Nigel Unwin	Experiments in electron microscopy: from metals to nerves (Gjønnes Medal lecture)
Hao Wu	Structural immunology and receptor signaling
Vittal Yachandra	Natural and artificial photosynthetic water oxidation
Jim De Yoreo	An in situ view of classical vs. non-classical pathways of nucleation and growth
Jihong Yu	Rational design and synthesis of inorganic microporous materials
Xiaodong Zou	Solving complex structures by electron crystallography

To participate in the
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*Crystallography helps to determine the ideal combination
of aluminium and magnesium in alloys used in aeroplane
manufacture. Too much aluminium and the plane will be too
heavy, too much magnesium and it will be more flammable.*
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IYCr2014 International outreach and some translated pages of "Crystallography matters!"

