The legacy of the International Year of Crystallography

*Under the High Patronage of His Majesty the King Mohamed VI*

**jointly organized by** International Union of Crystallography, IUCr
Moroccan Crystallographic Association, AMC

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**Building Capacity in Crystallography**

- History, Organization and Services of the IUCr
- IYCr 2014 Activities
- IUCr - Support for Building Capacity in Crystallography
1947 the IUCr, founded after an idea of P.P. Ewald, is accepted into ICSU
1948 the first elected President by the General Assembly is W.L. Bragg
1948 the first issue of *Acta Crystallographica* is released
promote international cooperation in crystallography

form a focus for the relations of crystallography to other sciences.

facilitate standardization of methods, units, nomenclatures and symbols

promote international publication of crystallographic research

contribute to the advancement of crystallography in all its aspects, including related topics concerning the non-crystalline state
IUCr Executive Committee plus – Leuven 2013

Front Row: Hanna Dabkowska, Luc Van Meervelt (Sec./Teas.), Marvin Hackert (President), Mike Glazer (Vice-Pres.), and Gautam Desiraju (Past-Pres.); Back Row: Malcolm Cooper (Fin. Comm.), Michael Dacombe (Exec. Sec.), Mitchell Guss, Radomir Kuzel, Masaki Takata, Wulf Depmeier, and Santiago Garcia-Granda.
53 member countries
42 adhering Bodies (including 4 regional Associates)
23 commissions
9 journals (IUCrJ launched in 2014)
IUCr Congress every 3 years:

23rd IUCr Congress, Montréal, August 2014
24th IUCr Congress, Hyderabad, India 2017
25th IUCr Congress, Praha, Czech Rep. 2020
Regional Associates of the IUCr

European Crystallographic Association (ECA), from 1978
Asian Crystallographic Association (AsCA), from 1987
American Crystallographic Association (ACA), from 1990
Latin American Crystallographic Association (LACA), from 2014
The scientific work of the IUCr is conducted primarily through its Commissions. Each Commission comprises a group of scientists who report to the Executive Committee on a particular subject area, maintain website, organize scientific sessions, etc.

Commission on Aperiodic Crystals
Commission on Biological Macromolecules
Commission on Charge, Spin and Momentum Densities
Commission on Crystal Growth and Characterization of Materials
Commission on Crystallographic Computing
Commission on Crystallographic Nomenclature
Commission on Crystallographic Teaching
Commission on Crystallography in Art and Cultural Heritage
Commission on Crystallography of Materials (*ad interim*)
Commission on Electron Crystallography
Commission on High Pressure
Commission on Inorganic and Mineral Structures
Commission on International Tables
Commission on Journals
Commission on Magnetic Structures
Commission on Mathematical and Theoretical Crystallography
Commission on Neutron Scattering
Commission on NMR Crystallography and Related Methods
Commission on Powder Diffraction
Commission on Small-Angle Scattering
Commission on Structural Chemistry
Commission on Synchrotron and XFEL Radiation
Commission on XAFS
IUCr journals
IUCr journals

Full open-access journals
The IUCr publishes two journals that are fully open access, i.e. all articles are made available free of charge to the reader. An open-access fee is charged to authors of articles published in these journals to cover the costs of peer review, journal production, and online hosting and archiving. These journals are:

- *Acta Crystallographica Section E: Structure Reports Online*
- *IUCrJ*

Hybrid open-access journals
Authors can choose to make their article open access by paying an open-access fee.

*Funds generated from open-access payments are used to keep subscription costs as low as possible.*

Waiving of open-access fees
Authors from developing countries may apply for their open-access fees to be waived. Also, Wiley has programs that provide free or low-cost on-line access to the journals in developing countries.
International Tables for Crystallography

Volume A  Space-group symmetry
Volume A1  Symmetry relations between space groups
Volume B  Reciprocal space
Volume C  Mathematical, physical and chemical tables
Volume D  Physical properties of crystals
Volume E  Subperiodic groups
Volume F  Crystallography of biological macromolecules
Volume G  Definition and exchange of crystallographic data
Volume H  Powder diffraction

to be released soon!
Published 4 times per year
Available online free of charge
Alerts sent to all those registered with the WDC
Circulated to over 200 different countries around the world

Contents
- Letters
- General news
- Awards
- Elections
- Useful resources and databases
- Event calendar and event reports
- Book reviews
- Comments and opinions
World Directory of Crystallographers
Facilitating communication within the crystallographic community

Launched in 1957, the database currently has 20,000 entries.

To sign-up is free, and members of the directory have access to a large network of scientists practising in similar and related fields of interest, tying together research topics, scientists and institutions in one easy to search database.

Ideal if you are looking for collaborators in other laboratories around the world or trying to find researchers with a general or detailed research background.

The database allows you to create your own unique profile, add your photo, research interests and papers published.

Manage subscriptions to journal e-alerts and the IUCr Newsletter from your profile, as well as enjoying the special offers on publications and services from time to time.
IUCr sponsorships

The IUCr currently sponsors scientific activities and meetings in a number of ways:

- Bursary scheme for meetings of Regional Associates
- Visiting Professorships
  The IUCr Visiting Professorship scheme aims to support some of the costs of having internationally recognized scientists as lecturers for short courses at workshops or schools organized in developing countries.
- Scientific conferences and workshops
- Journal subscriptions
- Crystallography in Africa
IUCr initiative

Crystallography in Africa

Approved by the IUCr Executive Committee following a proposal of Jan Boeyens from South Africa

- crystallography lecture series and schools
- bursaries awarded to African students to attend meetings of the IUCr Regional Associates
- bursaries for young professors (up to the age of 40), post-doctoral students and PhD students from Africa to attend an IUCr Congress
- instrumentation supplied free of charge by partner companies

Steering Committee
Claude Lecomte (Chair)
Patrice Kenfack
Luc Van Meervelt
Hocine Merazig
Romain Murenzi (TWAS)
Jean Paul Ngome (UNESCO)
Andreas Roodt
Abdelmalek Thalal
Michele Zema
IYCr Activities

✓ IUCr / IYCr web site - an educational resource for the future

http://www.iycr2014.org/timeline
Crystallography matters ... more!

✓ IUCr / IYCr web site - an educational resource for the future

- Declarations
- Reports
- News archive
- Media kit and coverage
- Videos
- Photo galleries
- PPT presentations
- Books
- Educational resources
- Collection of stamps
- Timelines of crystallography
- Crystallography365
- Gallery of crystals
- Partners
- New projects (to be continued)

... and quite a large facebook community
IYCr Activities

- Education - public awareness / outreach
Growing Crystals at Home

It is relatively easy and fun to grow crystals of common chemicals at home with a minimum of time and effort. Three of the favorite crystals to grow at home are alum (a common spice that can be obtained at most grocery stores), Borax (common detergent), and copper sulfate (used as a root killer). Crystals grow by a process termed nucleation from saturated or supersaturated solutions.

How much material it takes to make a saturated solution depends on the solubility of the substance. Most materials are more soluble in hot solutions, but the range varies a lot. For example, the solubility of common table salt (NaCl) increases by less than 10% between room temperature and the boiling point of water, whereas the solubility of copper sulfate increases by over 4-fold over this same temperature range (see graph below taken from Ref 1 Dom's crystal growing webpage).

There are many web links and YouTube videos to show you how to grow crystals at home. Below are just a few links to detailed steps on how to grow crystals at home. The alum crystal shown below at right was grown in less than 2 days.

Reference:

Dom’s crystal growing webpage: http://www.homepages.ucl.ac.uk/~uucraart/general/crystals.htm
About.com/chemistry/crystals facts: http://chemistry.about.com/od/crystalfacts/
About.com/crystal/recipes: http://chemistry.about.com/od/crystalfacts/crystalsrecipes.htm
Borax snowflake crystals: http://video.about.com/chemistry/Borax-Crystal-Snowflakes.htm
Large Alum crystals on youtube: http://www.youtube.com/watch?v=RayJkoS5EuA
Sodium acetate supersaturated solutions: http://www.youtube.com/watch?v=D1FDESoawwI
Bilateral symmetry, where the left and right sides are mirror images of one another, is common in nature such as seen in butterflies and snowflakes - and has also been a common feature of architecture.

Symmetry

Symmetry is integral to understanding crystals and crystallography. Something is symmetrical when it has similar parts: e.g., one part is the same as another part. The most common forms of symmetry are rotation axes and mirror planes. Symmetry can be observed all around us, even in our alphabet!

2-Fold Rotations

- 180° rotation about a vertical axis
- 180° rotation about a horizontal axis
- 180° rotation about an axis perpendicular to the page

Mirror Planes

- Vertical
- Horizontal

Now consider the alphabet shown below:

1) How many letters have no symmetry? ____. Place an “X” in the upper left box of letters with no symmetry.
2) How many letters have a vertical axis of symmetry? _____. Draw a vertical arrow indicating the symmetry axis.
3) How many letters have a horizontal axis of symmetry? _____. Draw a horizontal arrow indicating the symmetry axis.
4) How many letters are symmetrical about a 2-fold rotation axis perpendicular to the plane of the page? _____. Place a ( ) mark in the upper right box of those letters with a perpendicular 2-fold rotation axis, and a “dot” indicating the location of the rotation axis.
5) Now identify the symmetry present in the two words in the last two frames. Answers are given on the other side, but note results can vary with the font used!
IYCr Activities

✓ Building capacity – OpenLabs / workshops / summits
IYCr Activities - summits

- **Asia**: Karachi (Pakistan), 28-30 April 2014
  Vistas in Chemical crystallography

- **Latin America**: Campinas (Brazil), 22-24 Sept 2014
  Biological Crystallography and complementary techniques

- **Africa**: Bloemfontein (South Africa), 15-17 Oct 2014
  Crystallography as vehicle to promote Science in Africa and beyond
summit meetings
Karachi (Pakistan), 28-30 April 2014
Vistas in Structural Chemistry

Venue: International Center for Chemical and Biological Sciences (ICCBS), University of Karachi, Pakistan
Dates: 28-30 April 2014

Jointly organized by:
- Ministry of Science and Technology (MoST), Government of Pakistan
- Pakistan Academy of Sciences (PAS)
- Indian National Science Academy (INSA)
- Chinese Academy of Sciences (CAS)
- Commission on Science and Technology for Sustainable Development in the South (COMSATS)

Sessions
- Metal-Organic Framework Compounds (MOF)
- Crystal Engineering and Generic Pharmaceuticals
- Chemistry-Biology Interface and Drug Discovery and Designing
- Crystallography and complementary methods
- IUCr: Union & Journals
- Mini-Talks Session

Summit lecture
Prof Dr Atta-ur-Rahman, Promotion of higher education, science and technology and international cooperation in Pakistan

Three Panel discussions
We request the IUCr to initiate actions to promote regional scientific collaboration including ... leveraging national bodies and institutions for financial support and facilitating regional conferences on the subject of X-ray diffraction and its applications in the South Asian and East Asian regions.”
summit meetings

Campinas (Brazil), 22-24 September 2014

Biological Crystallography and Complementary Methods

Venue: Brazilian Synchrotron Light Laboratory (LNLS), Campinas, Brazil
Dates: 22-24 September 2014

Sponsored by:
- National Centre for Research in Energy and Materials
- Brazilian Synchrotron Light Laboratory
- Brazilian Bioethanol Science and Technology Laboratory
- Brazilian Biosciences National Laboratory
- Brazilian Nanotechnology National Laboratory
- Federal Government of Brazil

Sessions
- Historical Perspective on Protein Crystallography in Latin America
- Biological Crystallography
- Complementary Techniques
- A View from Abroad: Latin Americans Working Overseas

Keynote lecture
Ada Yonath  Can structures lead to advanced therapeutics?

Panel discussions
summit meetings
Campinas (Brazil), 22-24 September 2014
Biological Crystallography and Complementary Methods

“Through this letter, we request the IUCr and UNESCO to initiate actions to promote regional scientific collaboration including the holding of training workshops, encouraging the mobility of researchers within the region, promoting joint research projects, leveraging national bodies and institutions for financial support and facilitating regional conferences on the subject of X-ray crystallography and its applications in Latin America. We also request the IUCr to facilitate the establishment of a Latin American IYCr Cooperation Fund.”
Prof. Marvin Hackert, President, International Union of Crystallography
Prof. Lidia Brito, Regional Director, UNESCO

Dear Colleagues

24th September 2014

We are pleased to report that the IYCr Latin America Summit Meeting on Biological Crystallography in Campinas, Brazil during September 22-24, 2014, has provided us an opportunity to extensively discuss and review the status of education and research in X-ray diffraction sciences in various countries in the region.

Over 100 senior researchers, early career researchers, post-doctoral fellows and students from 12 countries have participated in the event including a number of well established scientists in the North (Europe and USA) with origins in the region. The reflections from these scientists regarding the level of regional collaboration indicated that this is clearly sub-optimal, suggesting the need to take immediate action.

Many of us were engaged in extensive discussions focusing on the promotion of regional and international cooperation in the field of X-ray crystallography and complementary methods, in line with the objectives of the International Year of Crystallography. These discussions were consistent with recent efforts leading to the founding of the Latin American Crystallographic Association (LACA). The venue, being the home of the first synchrotron light source in the southern hemisphere, was fitting, and served also to highlight the ambitions of the region in constructing one of the world’s most sophisticated, 4th generation light source, Sirius, before the end of the decade.

Through this letter, we request the IUCr and UNESCO to initiate actions to promote regional scientific collaboration including the holding of training workshops, encouraging the mobility of researchers within the region, promoting joint research projects, leveraging national bodies and institutions for financial support and facilitating regional conferences on the subject of X-ray crystallography and its applications in Latin America.

We also request the IUCr to facilitate the establishment of a "Latin American IYCr Cooperation Fund". We, as a community representative of our region, commit to persuade our academies, funding agencies and/or governments to provide annual contributions which are commensurate with each country’s economic reality. Our aim is to raise US $100K per annum for this fund. We request IUCr to provide encouragement by making an initial commitment of US $20K per annum for 3 years. We request IUCr/UNESCO to manage these funds.

The funds will be used for a variety of actions including:
1. increasing collaboration and cooperation among scientists of the region,
2. providing seed money for up to 2 projects per annum involving a minimum of 2 countries in the region, at least one of which should be well established in crystallography
3. funding for short term visits (up to 3 months), primarily aimed towards an Early Career Researcher,
4. training workshops at centres of excellence or emerging centres in the region,
5. enabling the sharing of facilities within the region.

Signed by all those present from the region

<table>
<thead>
<tr>
<th>NAME</th>
<th>position</th>
<th>Institution</th>
<th>Country</th>
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<tbody>
<tr>
<td>Hervínio Paez</td>
<td>Professor</td>
<td>Universidad de Chile</td>
<td>Chile</td>
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<tr>
<td>Daniel Espinosa</td>
<td>Professor</td>
<td>Universidad de Antofagasta</td>
<td>Chile</td>
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<tr>
<td>Roberto Cordero Paredes</td>
<td>Professor</td>
<td>Universidad de Chile</td>
<td>Peru</td>
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<tr>
<td>Sebastián Camacho Peña</td>
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<td>Universidad de Chile</td>
<td>Chile</td>
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<tr>
<td>Sebastian Klimek</td>
<td>Researcher</td>
<td>Instituto Leibniz</td>
<td>Argentina</td>
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<tr>
<td>Alejandro Alfaro</td>
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<td>Brookhaven National Lab</td>
<td>USA</td>
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<tr>
<td>M. Costabal</td>
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<td>Claudio Silva</td>
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<td>Juliane M.</td>
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<tr>
<td>José B. BC</td>
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</tr>
<tr>
<td>Bruno R. H.</td>
<td>Professor</td>
<td>Universidade de Brasília</td>
<td>Brasil</td>
</tr>
</tbody>
</table>

67 signatories follow
summit meetings

Bloemfontein (South Africa), 15-17 October 2014
Crystallography as vehicle to promote Science in Africa and beyond

Venue: Dept. of Chemistry, University of the Free State, Bloemfontein, South Africa
Dates: 15-17 October 2014

Jointly organized by:

University of the Free State, Bloemfontein, South Africa
South African Government’s Department of Science and Technology (DST)
European Crystallographic Association

9 Sessions
Young scientists flash presentations
3 Poster sessions
2 Panel discussions

Current state of Crystallography/Science in Africa
Way forward for crystallography/Science in Africa
summit meetings

Bloemfontein (South Africa), 15-17 October 2014

Crystallography as vehicle to promote Science in Africa and beyond

It provided the opportunity to consider, discuss and review the status of education and research on the broadly defined discipline of Crystallography in countries in the region.

- 100 senior researchers, early career researchers, post-doctoral fellows and students
- 40 research groups
- 32 universities
- 22 countries
The President: International Union of Crystallography
The Director of the Science Policy and Capacity Building Division: UNESCO
The President: European Crystallographic Association
The Commissioner of Human Resources, Science and Technology: Africa Union
All African Government Ministries of Science and Technology, Higher Education, Scientific research and Education

In celebration of 2014 as the International Year of Crystallography (IYCr) as declared by the United Nations General Assembly (UNGA; resolution A/RES/66/28), the International Union of Crystallography (IUCr) and UNESCO are leading the year-long activities.

With this document we are pleased to briefly report on the successful ‘Pan African Summit of the International Year of Crystallography 2014’ (IYCr2014Africa) in Bloemfontein, South Africa, 15-17 October 2014. It provided the opportunity to consider, discuss and review the status of education and research on the broadly defined discipline of Crystallography in countries in the region.

The conference and summit meeting was attended by more than 100 senior researchers, early career researchers, post-doctoral fellows and students representing more than 40 research groups from 32 universities and more than 20 countries, primarily from Africa and Europe, and included decision makers. The delegates were in agreement that there is clearly a sub-optimal level of regional collaboration which requires immediate action. It is our view that supporting the broad discipline of Crystallography will significantly contribute to promoting science in general.

We therefore request through this letter that the IUCr and UNESCO, supported by the European Crystallographic Association (ECA), but also in particular governments of African Countries and via the African Union and the International Council for Scientific Unions (ICSU), all initiate and support further actions to promote regional scientific collaboration. These include, but are not limited to, the following:

• pro-actively continue with programmes to ensure that the legacy of the International Year of Crystallography and particularly the promotion of science is preserved;

• over time provide basic diffraction equipment for crystallographers in all countries in the region to allow research activity in Crystallography and balanced partnership collaboration across Africa and beyond;

• facilitate the establishment of National Committees of Crystallography in African Countries and support the activities of the existing ones;

• introduce a scientific visa to ensure mobility of researchers between African nations. Such a visa would allow for the exchange and collaboration between African countries and the sharing of scientific resources and expertise, to address common developmental targets, for the benefit of all.

We further request that the IUCr and UNESCO facilitate the establishment of an African IYC r Cooperation Fund. As a community, we commit to engaging our local academies, funding agencies and/or governments to provide annual contributions commensurate with each country’s economic status. The aim is to raise 80 000 to 100 000 Euro per annum for this fund. We request the IUCr to commit to seed-funding of US$ 20 000 per annum for a three-year period. We further request the IUCr to manage these funds, or any local institution (such as AICA, once established) nominated by the IUCr.

The funds will support actions such as:

• increasing collaboration and cooperation among scientists in Africa;

• providing seed money for up to two projects per annum initially, involving a minimum of 2 countries in the region, of which at least one should be well established in Crystallography;

• funding for short term visits of up to 3 months for early career researchers;

• supporting training workshops at established centres of Crystallography or at emerging centres in the region;

• enabling the sharing of facilities within the region.

We envisage the formation of an African Crystallographic Association (AICA) to support and expand upon the actions above. A steering committee for this has been established at IYCr2014Africa in Bloemfontein.

These actions will enable Crystallography to be used in the promotion of science in the region and reiterate the need for immediate and well defined action.

Signed by those present,

73 signatories follow
summit meetings

Bloemfontein (South Africa), 15-17 October 2014

Appeal

- legacy of the International Year of Crystallography;
- provide basic diffraction equipment;
- establishment of National Committees of Crystallography;
- scientific visa;
- training workshops, education programmes, mobility of researchers, joint research projects, regional conferences;
- Formation of the African Crystallographic Association (AfCA).
summit meetings
Bloemfontein (South Africa), 15-17 October 2014

Appeal

We further request that the IUCr and UNESCO facilitate the establishment of an African IYCr Cooperation Fund. The funds will support actions such as:

- increasing collaboration and cooperation among scientists in Africa;
- providing seed money for up to two projects per annum initially, involving a minimum of 2 countries in the region, of which at least one should be well established in Crystallography;
- funding for short term visits of up to 3 months for early career researchers;
- supporting training workshops at established centres of Crystallography or at emerging centres in the region;
- enabling the sharing of facilities within the region.

We further request the IUCr to manage these funds, or any local institution (such as AfCA, once established) nominated by the IUCr.

We envisage the formation of an African Crystallographic Association (AfCA) to support and expand upon the actions above. A steering committee for this has been established at IYCr2014Africa in Bloemfontein.
ICSU Grants Programme 2015

Project title: *Building Science Capacity in Africa via Crystallography*

Lead Applicant: IUCr
Co-Applicant: ECA

Proposers: *Michele Zema* (IUCr), *Andreas Roodt* (ECA)

Supporting organizations: ECA, UNESCO, SAASTA, ICSU ROA, INDABA

**Project plan (2015/2016):**

1. *Follow-up meeting to the Bloemfontein Summit (to be held in North Africa)*
2. *Crystallography workshop in Central Africa* (preferably, DR Congo)
3. *Support to African scientists to attend the INDABA series of conferences in South Africa*

+ many additional actions
The IYCr legacy

✓ Building capacity / on-going training
✓ Set up the IYCr legacy fund
✓ Develop sustainable programmes in Africa, Asia and South America in collaboration with UNESCO and other international organization (e.g., TWAS, ICSU)
✓ Transition of other IYCr activities to sustainable long-term IUCr initiatives in collaboration with the national and regional associates
✓ Sustain the formation and development of new regional (LACA, AfCA) and national associations
✓ Create joint programs with large-scale facilities for students from the developing countries
✓ Integrate IYCr web site resources into a re-designed IUCr web site
Acknowledgements

- Organizers: Abdelmalek Thalal, Claude Lecomte, Michele Zema
- UNESCO / ICSU ROA / TWAS
- Moroccan Crystallographic Association (UN delegation)
- Academie Hassan II des Science & Techniques
- Industrial partners
- Chester Staff (Michele Zema – Project Manager for IYCr2014)
- Regional Associates
IYCr2014 Supporters
IYCr2014 Supporters: large-scale facilities