Crystallography working across nations

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Editor-in-Chief of IUCr journals
& Founding Editor of Journal of Synchrotron Radiation

1948
Acta Crystallographica launched
Founding editor: P.P. Ewald

66 years
2014

IUCrJ -100 years from FIRST Nobel prize to Crystallography

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IUCr facts

53 member countries

42 Adhering Bodies (including 4 Regional Associates: ACA, AsCA, ECA, LACA)

23 Commissions

9 Journals (including IUCrJ launched in 2014)

IUCr Congress every 3 years (24th IUCr Congress, Hyderabad, August 2017)

The IUCr is a member of ICSU since 1947
1948
Acta Crystallographica launched
Founding editor: P.P. Ewald

1968
Acta Crystallographica split into
Section A: Foundations of
Crystallography and Section B:
Structural Science
Founding editor: A.J.C. Wilson

1968
Journal of Applied Crystallography
launched
Founding editor: A. Guinier

1983
Acta Crystallographica Section C:
Crystal Structure Communications
launched
Founding editor: S.C. Abrahams

1991
Adoption of CIF

1993
Acta Crystallographica Section D:
Biological Crystallography
launched
Founding editor: J.P. Glusker

1994
Journal of Synchrotron
Radiation launched
Founding editors:
S.S. Hasnain, J.R. Helliwell
and H. Kamitsubo

1999
Online access

2001
Acta Crystallographica Section E:
Structure Reports Online launched
Founding editors: W. Clegg
and D.G. Watson

2002
Back issues online

2005
Acta Crystallographica Section F:
Structural Biology and
Crystallization Communications
launched
Founding editors:
H.M. Einspahr and J.M. Guss

2014
IUCrJ to be launched
Founding editors: E.N. Baker, G.R. Desiraju,
C.R.A. Catlow, S. Larsen and J.C.H. Spence
The new open-access high-influence journal from the IUCr [www.iucrj.org](http://www.iucrj.org) to celebrate the International Year of Crystallography

Complete studies reported as Research Articles (7000 words) and Letters (4000 words).

Submit your outstanding work & become part of heritage [www.iucrj.org/m/services/submit.html](http://www.iucrj.org/m/services/submit.html)

Second Year of outstanding papers!
Some example of papers published in 2014 in IUCrJ

BIOLOGY | MEDICINE
Open access

CHEMISTRY | CRYSTENG
Crystal landscape in the orcinol:4,4′-bipyridine system: synthon modularity, polymorphism and transferability of multipole charge density parameters
*Ritesh Dubey,* a **Mysore S. Pavan,** a **Tayur N. Guru Row** a* and **Gautam R Desiraju** a*

PHYSICS | FELS
*Ab-initio* phasing using nanocrystal shape transforms with incomplete unit cells
*Haiguang Liu,* a **Nadia A. Zatsepin** a and **John C. H. Spence** a*

MATERIALS | COMPUTATION

NEUTRON & SYNCHROTRON
The Collaborative Computational Project Number 4 in Protein Crystallography was set up in 1979 to support collaboration between researchers working on method and software development for Protein Crystallography in the UK. It soon expanded to become a global example of collaboration and has been one of the contributory factor for Biological Crystallography. Since 1998 ACTA CRYST D is publishing latest efforts that are reported at the annual CCP4 study weekends.
Michael Rossmann, Eleanor Dodson, Phil Evans

CCP4 Conference Study Weekend
January 2000
York University

Phil Burke

STFC Daresbury Laboratory
The Synchrotron Radiation Source (SRS) at Daresbury (Cheshire, UK) was the world’s first dedicated Synchrotron X-ray Source. It came operational in 1980 and was closed in October 2008.

SR Light

Opening angle $\Theta = \frac{mc^2}{E}$

The layout of a wiggler
30 years from NINA SRF

World’s largest storage ring started in 1997 (Spring-8 in Japan)

50 years since the first observation of SR by Blewett

Many of us discussed privately at the time that SR world had expanded beyond our imagination but the ultimate prize had not yet come. In 1997, first prize came – John Walker, followed by several SR related Nobel prizes [McKinnon(2003), Kornberg (2006); Steitz, Ramakrishnan & Yonath (2009); Kobilka (2012). 2nd X-ray laser started (SACLA) in 2012 – 100 years after Laue & Bragg discoveries.
A comparison of peak spectral brightness $B_n^{\text{peak}}$ [see equation (14)] of some storage-ring and FEL sources. Reprinted with permission from Schmüser et al. (2014).

\[ B_n^{\text{peak}} = \frac{B_n}{f_b t_b}, \quad (14) \]

where $f_b$ and $t_b$ are the pulse frequency and duration, respectively.
1 Å

1 nm

10 nm

100 nm

1 µm

10 µm

visible rays

UV rays

soft X-rays

X-rays

hard X-rays

long wavelength (low energy) ← [wavelength] → short wavelength (high energy)

Synchrotron Light

Lamps

X-ray Tubes

XFELs

another >10 billion in peak
Highlights of the Many Nobel Prizes Awarded to Crystallographers

1901
Wilhelm Röntgen
Discovery of X-rays

1914
Sir William H. & Sir William L. Bragg
First X-ray crystal structure

1917
Barkla

1915
Max von Laue
First demonstrated X-ray diffraction through crystals

1926
Max Perutz
Hemoglobin

1944
Francis Crick, James Watson & Maurice Wilkins
Created DNA model double-helical structure for biological information storage

1962
Dorothy Hodgkin
The structure of vitamins, cholesterol, penicillin, vitamin B12, and insulin

1964
William Lipscomb
The structure of boranes, illuminating problems of chemical bonding

1976
Max Perutz & Sir John Kendrew
Haemoglobin and muscle protein structures

1985
Herbert Hauptman & Jerome Karle
Direct methods of determining crystallographic structures

1988
John Deisenhofer, Robert Huber & Hartmut Michel
First membrane protein, which is essential to photosynthesis

1994
C. B. Fermi & Bertram Brockhouse
Electron diffraction and neutron diffraction

2001
Den Shchaken
Discovery of quasicrystals

2009
Yoshihito Morikawa, Tom Steitz & Ada Yonath
Studies of the structure and function of the ribosome

2011
Rod McKinnon
Discovery of quasicrystals

2013
Martin Karplus, Michael Levitt & Arieh Warshel
Development of sophisticated computer simulations for complex chemical processes

Six most Recent Nobel prizes in Biological Crystallography most related to synchrotron radiation

John Walker – 1997
Tom Steitz, Venki Ramakrishnan & Ada Yonath – 2009
Rod McKinnon – 2003
Brian Kobilka – 2012
Roger Kornberg – 2006
Karplus, Levitt & Warshall – 2013

Issued by Royal Mail on 25 March 2014
It is clear that Crystallography and Synchrotron light have brought global community of structural scientists from physics, chemistry and biology background creating many cross-disciplinary fields removing the ‘traditional’ boundaries of disciplines. The widespread use of these is a testimony of success of bringing nations together pushing the scientific frontiers as well as overcoming geo-political limits.
SESAME = Synchrotron-light for Experimental Science and Applications in the Middle East


**Members**
Bahrain, Cyprus, Egypt, Israel, Iran, Jordan, Pakistan, Palestinian Authority, Turkey

**Purpose:** Foster excellent science and technology in the Middle East, and prevent or reverse the brain drain, by enabling world-class research in subjects ranging from biology and medical sciences through materials science and physics to archaeology.

*Build bridges between diverse societies and contribute to a culture of peace through international cooperation in science.*
Contributing to Fulfill Dreams of next generation of Scientists from the region – From Oct 2010, started PhD at the University of Copenhagen in Medicinal Chemistry – completed PhD in 2014.

November 23, 2009

Rt Hon David Miliband
Foreign Secretary
Her Majesty’s Government of the United Kingdom

I am currently with Professor Samir Hasnain from the University of Liverpool at the SESAME users meeting in Jordan, which is attended by young and senior scientists from member countries including Iran, Israel, Pakistan, Turkey, Cyprus, Egypt, and Jordan. I understand that you have learnt recently about SESAME, a project established under the sponsorship of UNESCO, from Professor Hasnain. SESAME is an advanced synchrotron facility like DIAMOND in your country. At the latest User’s meeting from where I am writing this letter, it is heartening to see how this project is bringing the scientists and Governments’ representatives of the member countries together working hard to achieve their dream of establishing this advanced facility in the region. I write to you as I feel that without engagement of countries like UK and USA, the project may not get completed for a long time.
Scientific thought is the common heritage of all mankind (Abdus Salam, 1986)
Some salient points relevant to the Summit meetings are worth noting.

“International relations is experiencing its own “Quantum” shift. ... And in this new world, more than any other that has gone before, I believe that science has a vital role to play in international relations and diplomacy”.

“In Europe, CERN helped rebuild links between nations - establishing the first post war contacts between German and Israeli scientists and keeping open relations between Western and Eastern Europe.”

“Science can and should be used to break down barriers of the twenty-first century, particularly those between the Western and Muslim-majority countries. Projects like the new Synchrotron light-source (SESAME) in Jordan are leading the way, bringing together scientists from Bahrain, Cyprus, Egypt, Israel, Iran, Jordan, the Palestinian Authority, Turkey and Pakistan to build a bright light-source for cutting-edge experiments in materials science and biology.”
The Summit Meetings will stress high-level science and also highlight the problems and difficulties in conducting competitive scientific research in several parts of the world. They are also aimed at discussing the actual possibilities for developing crystallographic research and technology in those regions.
IYCr2014 LATIN AMERICA SUMMIT DECLARATION
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
Through this letter, we request the IUCr to initiate actions to promote regional scientific collaboration including joint holding of training workshops, video-based lecturing, encouraging mobility of researchers, promoting joint research projects, 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.

PAKISTAN BECAME A MEMBER IN AUG 2014. CHINA, INDIA and PAKISTAN (CATEGORY 4, 3 & 1)
## 22 IUCr Presidents in 66 years from 11 countries fostering collaboration

<table>
<thead>
<tr>
<th>Year Range</th>
<th>President</th>
<th>Country</th>
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<tbody>
<tr>
<td>1948-1951</td>
<td>Sir Lawrence Bragg</td>
<td>UK</td>
</tr>
<tr>
<td>1951-1954</td>
<td>J.M. Bijvoet</td>
<td>The Netherlands</td>
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<tr>
<td>1954-1957</td>
<td>R.W.G. Wyckoff</td>
<td>USA</td>
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<tr>
<td>1957-1960</td>
<td>J. Wyart</td>
<td>France</td>
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<tr>
<td>1960-1963</td>
<td>P.P. Ewald</td>
<td>USA</td>
</tr>
<tr>
<td>1963-1966</td>
<td>J.D. Bernal*</td>
<td>UK</td>
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<tr>
<td>1966-1969</td>
<td>N.V. Belov</td>
<td>USSR</td>
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<tr>
<td>1972-1975</td>
<td>D. Hodgkin</td>
<td>UK</td>
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<tr>
<td>1975-1978</td>
<td>A. Magnéli</td>
<td>Sweden</td>
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<tr>
<td>1978-1981</td>
<td>N. Kato</td>
<td>Japan</td>
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<tr>
<td>1981-1984</td>
<td>J. Karle</td>
<td>USA</td>
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<tr>
<td>1987-1990</td>
<td>M. Nardelli</td>
<td>Italy</td>
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<tr>
<td>1990-1993</td>
<td>A. Authier</td>
<td>France</td>
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<tr>
<td>1993-1996</td>
<td>P. Coppens</td>
<td>USA</td>
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<tr>
<td>1996-1999</td>
<td>E.N. Baker</td>
<td>New Zealand</td>
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<tr>
<td>1999-2002</td>
<td>H. Schenk</td>
<td>The Netherlands</td>
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<tr>
<td>2002-2005</td>
<td>W.L. Duax</td>
<td>USA</td>
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<tr>
<td>2005-2008</td>
<td>Y. Ohashi</td>
<td>Japan</td>
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<tr>
<td>2008-2011</td>
<td>S. Larsen</td>
<td>France</td>
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<tr>
<td>2011-2014</td>
<td>G.R. Desiraju</td>
<td>India</td>
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*Just before the Seventh General Assembly in 1966, the then President, J.D. Bernal, resigned for reasons of health. Dame Kathleen Lonsdale (UK) assumed the office of President until the close of the Seventh General Assembly.*
Science and technology are cyclical. They are a shared heritage of all mankind. East and West, North and South have all equally participated in their creation in the past, as we hope that they will in the future – the joint endeavor in sciences becoming one of the unifying forces among diverse peoples of this globe.

Muhammad Abdus Salam
Science and Technology Education in the Development of the South
Prepared for the South Commission September 1990
Third World Academy of Sciences

IYCr, I hope, will be remembered for bringing nations together creating opportunities for younger generations from all parts of the globe to pursue the best of Crystallography independent of their location, ethnicity, religion or race.