### **Crystallography working across nations**

1948

**IUCr** 

Acta Crystallographica launched Founding editor: P.P. Ewald



66 years

2014

### Samar Hasnain

Max Perutz Professor of Molecular Biophysics, University of Liverpool, UK

# Editor-in-Chief of IUCr journals

Founding Editor of Journal of Synchrotron Radiation

Volume 68 (January 2012)



Acta Crystallographica Section A

Volume 69, Part 1 (January 2013)



IUCrJ -100 years from FIRST Nobel prize to Crystallography

100 years of Crystallography



s.s.hasnain@liverpool.ac.uk & Samar.hasnain@iucr.org



member countries

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

Commissions

IUCr Congress every

Journals (including IUCrJ launched in 2014)

years (24<sup>th</sup> IUCr Congress, Hyderabad, August 2017)

The IUCr is a member of ICSU since 1947

# **IUCr Journal milestones**



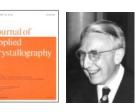
1948

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



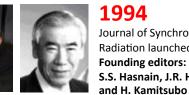
1983 Acta Crystallographica Section C: **Crystal Structure Communications** launched Founding editor: S.C. Abrahams

1991 Adoption of CIF



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





#### Journal of Synchrotron Radiation launched Founding editors: S.S. Hasnain, J.R. Helliwell

1999 Online





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



Vislame 1 | Part 1 | 1 January 2014 | Pages 1-106



International Union of CRYSTALLOGRAPHY The new open-access high-influence journal from the IUCr <u>www.iucrj.org</u> 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

# Second Year of outstanding papers !



158N 2052-2525

# Some example of papers published in 2014 in **IUCrJ**

BIOLOGY | MEDICINE

Open access

 <u>Structure and function study of the complex that synthesizes S-adenosylmethionine. B.</u> <u>Murray</u>, <u>S. V. Antonyuk</u>, <u>A. Marina</u>, <u>S. M. Van Liempd</u>, <u>S. C. Lu</u>, <u>J. M. Mato</u>, <u>S. S. Hasnain</u> & <u>A. L. Rojas</u> (2014). *IUCrJ* 1, 240-249.

#### CHEMISTRY | CRYSTENG

Crystal landscape in the orcinol:4,4'-bipyridine system: synthon modularity, polymorphisr and transferability of multipole charge density parameters

<u>Ritesh Dubey, a Mysore S. Pavan, a Tayur N. Guru Rowa</u> and <u>Gautam R Desirajua</u>

#### PHYSICS | FELS

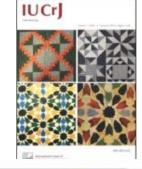
*Ab-initio* phasing using nanocrystal shape transforms with incomplete unit cells <u>Haiguang Liu,<sup>a</sup> Nadia A. Zatsepin<sup>a</sup></u> and <u>John C. H. Spence<sup>a\*</sup></u>

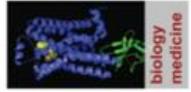
#### MATERIALS | COMPUTATION

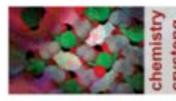
<u>The first X-ray diffraction measurements on Mars. D. Bish</u>, <u>D. Blake</u>, <u>D. Vaniman</u>, <u>P. Sarrazin</u>, <u>T. Bristow</u>, <u>C. Achilles</u>, <u>P. Dera</u>, <u>S. Chipera</u>, <u>J. Crisp</u>, <u>R. T. Downs</u>, <u>J. Farmer</u>, <u>M. Gailhanou</u>, <u>D. Ming</u>, <u>J. M. Morookian</u>, <u>R. Morris</u>, <u>S. Morrison</u>, <u>E. Rampe</u>, <u>A. Treiman</u> & <u>A. Yen</u> (2014). *IUCrJ* 1, 514-522.

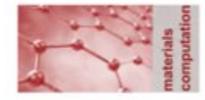
#### **NEUTRON & SYNCHROTRON**

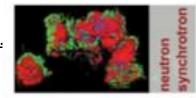
 <u>X-ray techniques for innovation in industry</u>. K. Lawniczak-Jablonska & J. Cutler (2014). IUCrJ 1, 604-613.

















Phil Burke Tom Blundel







Late David Blow Ta

Talapady N. Bhat

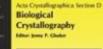
The Collaborative Computational Project Number 4 in Protein Crystallography was set up in 1979 to support collaboration between researchers working on method and software development for Protein Crystallography in the UK. It soon expanded to become a global example of collaboration and has been one of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



cta Crystallingraphica Section D Biological Crystallography ditor (may P. Chailer



1999









eta Oystallographica Section D Biological Crystallography Idinary F. N. Baker and Z. Dawler



2003



Phil Burke



CCP4 Conference Study Weekend January 2000 York University

Michael Rossmann, Eleanor Dodson, Phil Evans



Acta Crystallingraphica Section D Biological Crystallography Iditors E. N. Baker and Z. Danker

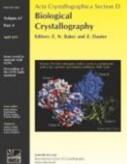


2007

eta Oystallographica Section D Biological Crystallography diters E. N. Baker and Z. Danks



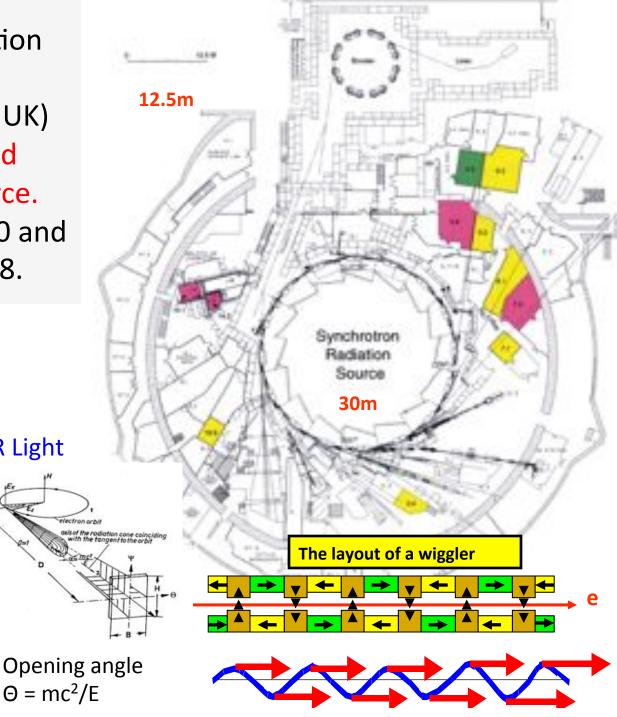
2009



2011

The Synchrotron Radiation Source (SRS) at Daresbury (Cheshire, UK) World's first dedicated Synchrotron X-ray Source. Came Operational in 1980 and closed in October 2008.





### 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

Editorial

### JSR, 4, 315 (1997)

J. Synchrotron Rad. (1997). 4, 315

#### Fifty Years of Synchrotron Radiation

#### S. Samar Hasnain,<sup>a</sup> John R. Helliwell<sup>b</sup> and Hiromichi Kamitsubo<sup>c</sup>

This issue marks the 50th anniversary of the first observation of synchrotron radiation light from the General Electric 70 MeV synchrotron and coincides with the third anniversary of the *Journal of Synchrotron Radiation (JSR)*. The issue brings together review articles from some of the pioneers of the field and in our view forms a unique historical record.





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). 2<sup>nd</sup> X-ray laser started (SACLA) in 2012 – 100 years after Laue & Bragg discoveries.



IUCLJ ISSN 2052-2525 NEUTRON SYNCHROTRON The potential of future light sources to explore the structure and function of matter

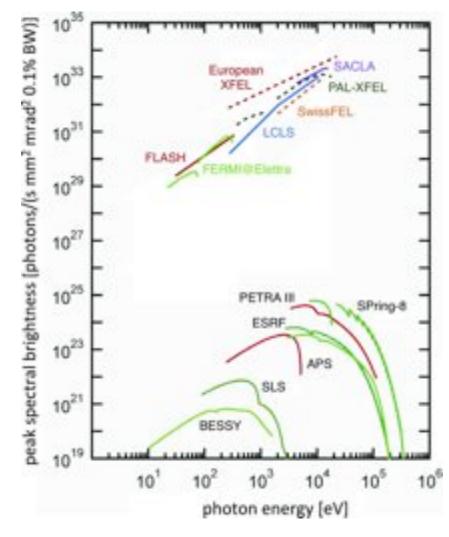
Edgar Weckert\*

A comparison of peak spectral brightness B<sub>n</sub><sup>peak</sup> [see equation (14)] of some storage-ring and FEL sources. Reprinted with permission from Schmüser et al. (2014).

$$B_n^{\text{peak}} = \frac{B_n}{f_b t_b},\tag{14}$$

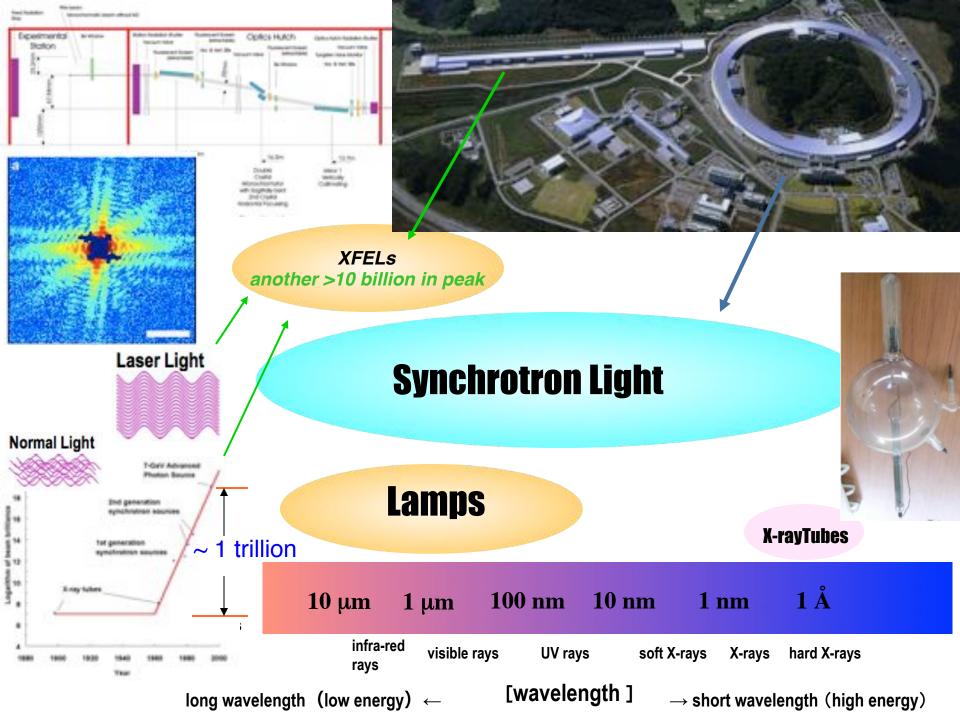
where  $f_b$  and  $t_b$  are the pulse frequency and duration, respectively.





#### Weckert

Volume 2 | Part 2 | March 2015 | Pages 230–245 | 10.1107/S2052252514024269







1954

Withelm Rånger Discovery of X-rays

1901

Aphs-Nelical MANAGER OF Prance Crick, James Watson & Maurice Wilking proteins, nature of Created DNA model double-helical structure chemical bonds for biological information storage

1962

**Highlights of the Many Nobel Prizes** Awarded to Crystallographers

1985



See a complete list of winners at luctorg/people/nobel-prize



quasicrysteals

2011

1917 BARKLA

Mox von Laue Sir William H. & First demonstrated SerWilliam L Brugg X-ray diffraction. First atomic







John Kendrew & Mile Peruta

Hemoglubin Transport

Max Penala 1914 - 2002 Molecular biologist and Nobel Iver issued by Royal Mail on 25 March 2014

1976

**Density Hodgkin** William Lipscomb Structures of The structure of protein, which led to cholesterol. **boranes** Illuminating periolity, vicenie problems of Sickle Cell-Anenta 812 and insulin chemical bonding





2003

neutron diffraction

994

Rager Kamberg Soudies of the molecular basis of eukaryotic transcription.







function of the ribosome

2009



Martin Karplus, Michael Loviti

Development of apphinistant

complex chemical processes

& Ariel: Warshell

computer simulations for 2013





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lands History Applied Pallemeter's map to libertify planes and severan in different dates in allest interconting

Six most Recent Nobel prizes in Biological Crystallography most related to synchrotron radiation John Walker – 1997 Tom Steitz, Venki Ramakrishnan & Ada Yonath – 2009

Peter Apre

& Roderick

MacKinness

membranes

Rod McKinnon – 2003 Brian Kobilka – 2012 Roger Kornberg – 2006 Karplus, Levitt & Warshall –2013

It is clear that Crystallography and Synchrotron light have brought global community of structural scientists from physics, chemistry and biology background creating many crossdisciplinary 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

(2.5 GeV light source). A major facility, under construction near Amman.



Members Bahrain, Cyprus, Egypt, Israel, Iran, Jordan, Pakistan, Palestinian Authority, Turkey SESAME building, financed by Jordan and designed by civil engineers from Al-Balqa' Applied University, Jordan



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.



Ada Yonath, Pro The Martin S. and Professor of Struc Director, The Hole Kimmelman Cent Structure and Ass http://www.w

November 23, 2009

Rt Hon David Milliband Foreign Secretary Her Majesty's Government of the United Kingd

I am currently with Professor Samar 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 lran, 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.

A photo with a young scientist from Iran who spent three months at the University of Liverpool in 2009 under SESAME training programme. November 2009



# IUCrJ Summit meetings IYCr2014





United Nations Educational, Scientific and Cultural Organization

### international year of crystallography

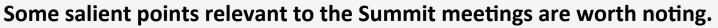


International Union of Crystallography

### www.iycr2014.org

## Scientific thought is the common heritage of all mankind (Abdus Salam, 1986)

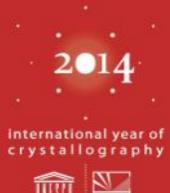




"International relations is experiencing its own "Quantum" shift. ... And in this new world, more than any other that has gone before, I believe that science has a vital role to play in international relations and diplomacy".

"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."



### Little faith and the second se

when for the transmissional Year of Crystallography 2014

# summit meetings intra-region cooperation

# bringing nations together

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

 Latin America: Campinas (Brazil), 21-24 September 2014, Biological Crystallography and complementary techniques
<u>Africa</u>: Bloemfontein (South Africa), 15-16 October 2014, Materials Science and Mining

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 DACLARATION



#### Prof. Marvin Hackert, President, International Union of Crystallography Prof. Lidia Brito, Regional Director, UNESCO

#### **Dear Colleagues**

#### 24<sup>th</sup> 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



IYCr2014 South Asia Summit Meeting on Vistas in structural chemistry

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



1948-1951 Sir Lawrence Bragg UK



1951-1954 J.M. Bijvoet The Netherlands



1954-1957 R.W.G. Wyckoff USA



1957-1960 J. Wyart France



1960-1963 P.P. Ewald USA



1963-1966 J.D. Bernal\* UK



1966-1969 N.V. Belov

1969-1972

A. Guinier

1972-1975

France



1984-1987 Th. Hahn Germany, Fed. Rep.



1987-1990 M. Nardelli Italy



1990-1993 A. Authier France

1996-1999

E.N. Baker

New Zealand

1993-1996 P. Coppens USA





1999-2002 H. Schenk The Netherlands



2002-2005 W.L. Duax USA



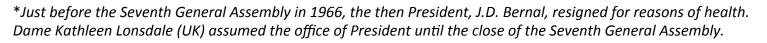
2005-2008 Y. Ohashi Japan



2008-2011 S. Larsen France



2011-2014 G.R. Desiraiu India





1975-1978 A. Magnéli Sweden

1978-1981

1981-1984

J. Karle

USA

N. Kato Japan

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.