CRYSTALLOGRAPHY AND SUSTAINABILITY

John R. Helliwell
School of Chemistry, University of Manchester, UK
john.helliwell@manchester.ac.uk

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Transactions Symposium

What precisely is 'sustainability' and how might we fit into it?

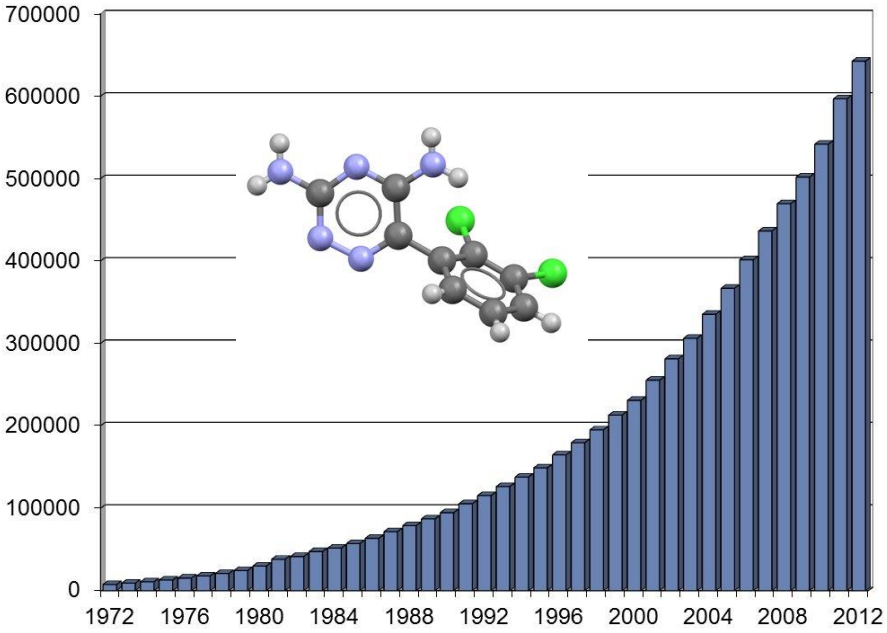
- *"The world's sustainable development goals are integrated into the eight **Millennium Development Goals** (**MDGs**) that were established in 2000 following the Millennium Summit of the United Nations. Adopted by the 189 United Nations member states at the time and more than twenty international organizations, these goals were advanced to help achieve the following sustainable development standards by 2015:*
- *To eradicate extreme poverty and hunger*
- *To achieve universal primary education*
- *To promote gender equality and empower women*
- *To reduce child mortality*
- *To improve maternal health*
- *To combat HIV/AIDS, malaria, and other diseases*
- *To ensure environmental sustainability*
- *To develop a global partnership for development"*

Reference: http://en.wikipedia.org/wiki/Sustainability

Talk contents

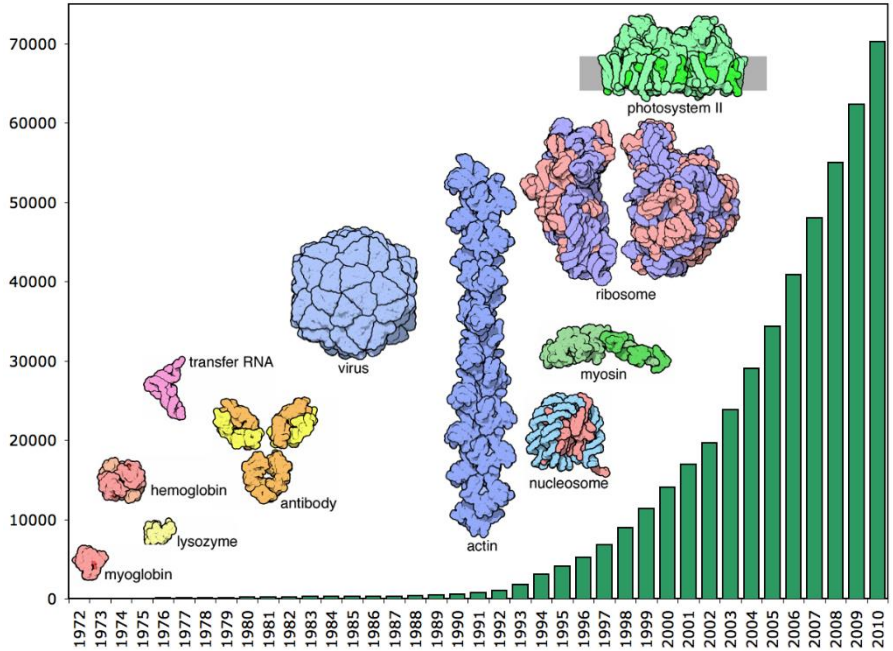
- Research and Knowledge Transfer
- Nanomaterials
- Overarching publications and access to data policy and the principle of open access
- Databases
- Green chemistry: “doing more with less and less pollution”
- Capacity building in our crystallographic World
- Conclusions

Fruits of our research: Structures large and small



Cambridge Structural Database

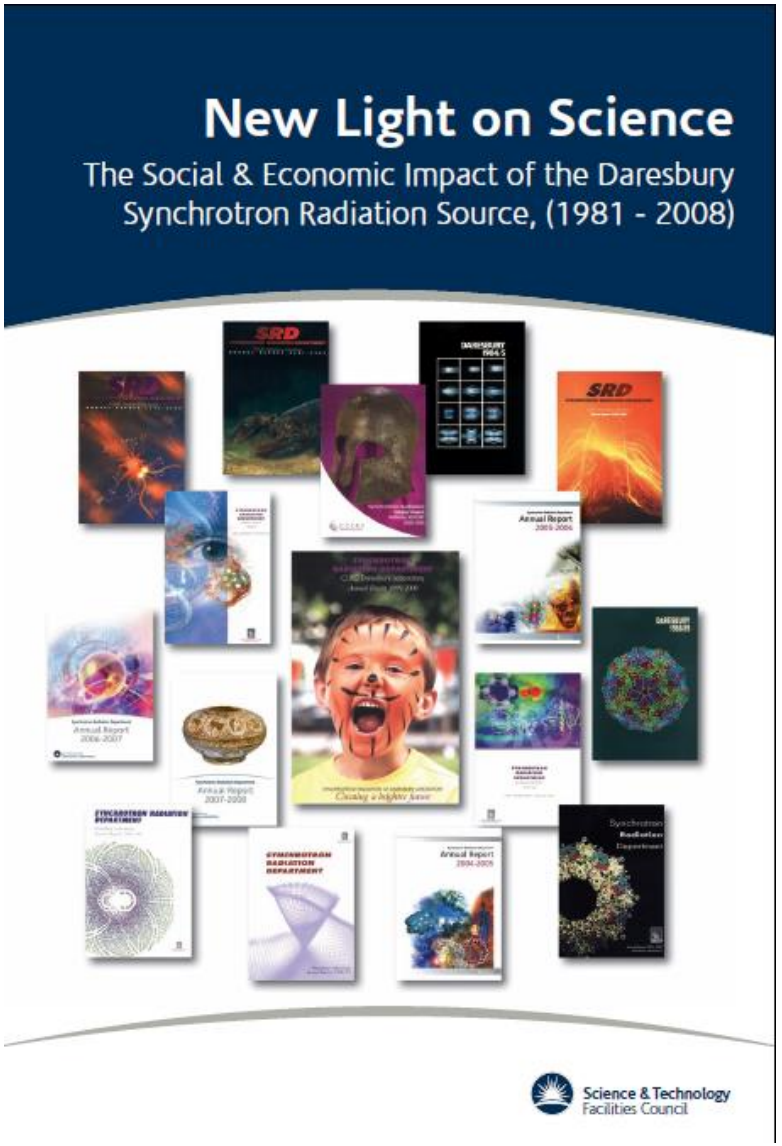
686944 structures at 6 January 2014



Protein Data Bank

104371 structures at 23 October 2014

Knowledge Transfer: ***Daresbury Analytical and Research Technical Services*** (DARTS); an important aspect of the Economic Impact of the SRS



E.J. Maclean, P.J. Rizkallah and J.R. Helliwell (2006) Protein Crystallography and Synchrotron radiation European Pharmaceutical Review Issue 2, p71-76

Approx £300k income to SRS per annum;

Australia and Canada each pushed on the usual ceiling of a ‘10% maximum’ commercial use.

IUCr was invited to participate in a CODATA / VAMAS Working Group in 2012

- VAMAS is the Versailles Project on Advanced Materials and Standards (www.vamas.org). There have been 3 Workshops so far.

- The overall goal is to define the needs of as many scientific disciplines and user communities as possible. This White Paper will be transmitted to ISO Technical Committee 229 on Nanotechnology (http://www.iso.org/iso/iso_technical_committee?commid=381983) as well as other international and national standards development bodies and government agencies. Within this Working Group, Crystallographers unambiguously define and characterize nanomaterials.

CODATA/VAMAS Nanomaterials project; IUCr's input

Crystallography Information File (CIF)

CIF dictionaries provide a formal taxonomy of crystallographic terms and ideas. Dictionary entries are constructed in a structured machine-readable manner that facilitates validation and structuring of data: http://www.iucr.org/resources/cif/dictionaries

Dictionaries: Core, Restraints, Powder, Modulated-Composite, Electron density, Twinning, Macromolecular, Images, Symmetry

Local dictionnaries: reflectivity (to come), MPOD (Properties), MAUD

Crystallographic Techniques

Diffraction (scattering + interferences): X, γ, n, e^-

Reflectivity (specular, off-specular): x-rays and neutrons

Small-Angles Scattering: x-rays (SAXS), neutrons (SANS)

Tomography (absorption or phase contrasts): x-rays, neutrons, electrons

Spectroscopy: X (XRF, XANES, EXAFS, DAFS)
e^- (EDS)
μ^+ (μSR)

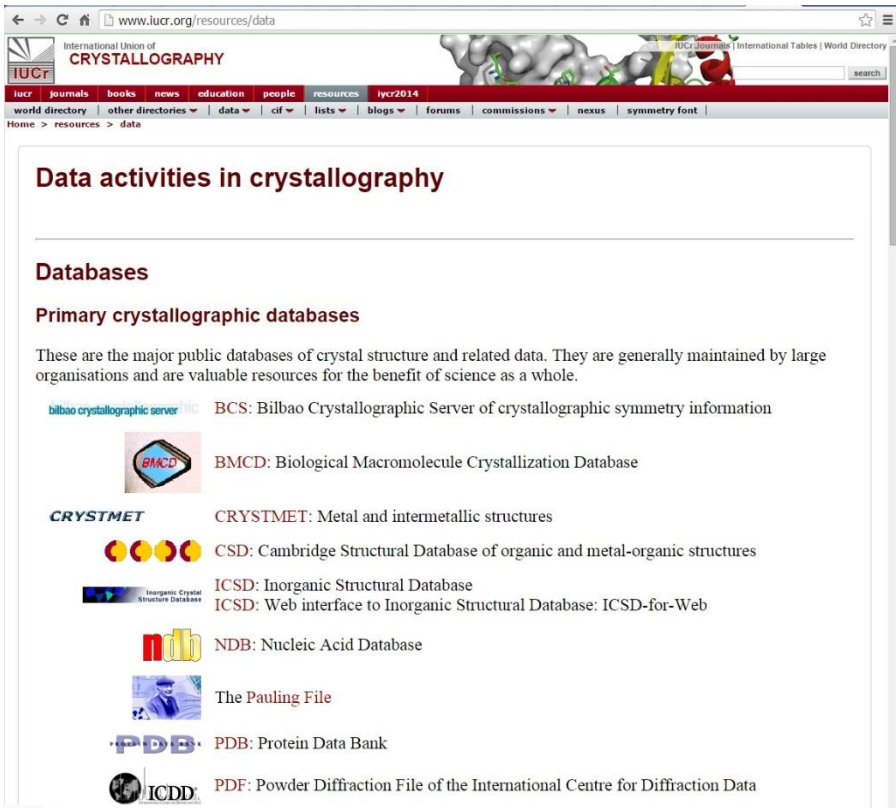
Overarching data policy and the principle of open access

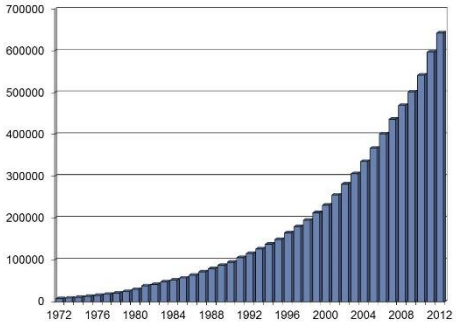
- http://www.icsu.org/general-assembly/news/ICSU%20Report%20on%20Open%20Access.pdf
- *"The International Council for Science advocates the following goals for open access. The scientific record should be:*
    - *free of financial barriers for any researcher to contribute to;*
    - *free of financial barriers for any user to access immediately on publication;*
    - *made available without restriction on reuse for any purpose, subject to proper attribution;*
    - *quality-assured and published in a timely manner; and*
    - *archived and made available in perpetuity.*

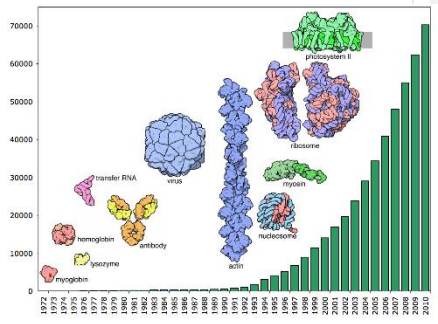
** These goals apply both to peer-reviewed research publications, the data on which the results and conclusions of this research are based, and any software or code used in the course of the research."*

Benefits of retaining derived data

- Scientific record
- Database-driven discovery
- Protein-ligand interactions
- New pathways to synthesis, manufacturing, energetics…
- Identification/indexing (*e.g.* forensic science)







Benefits of retaining processed data

- Structure validation
- Re-refinement
- Systematic bias, methods development
- Guard against structures associated with incorrect data sets

journals.iucr.org/b/issues/2002/01/00/bm0047/index.html

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Structural Science

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Some 60 new space-group corrections

Richard E. Marsh,[a] Moshe Kapon,[b] Shengzhi Hu[c] and Frank H. Herbstein[b]*

[a]The Beckman Institute, California Institute of Technology, Pasadena, CA 91125, USA, [b]Department of Chemistry, Technion-Israel Institute of Technology, Haifa 32000, Israel, and [c]Department of Chemistry, Xiamen University, Xiamen, Peoples' Republic of China
Correspondence e-mail: chr03fk@tx.technion.ac.il

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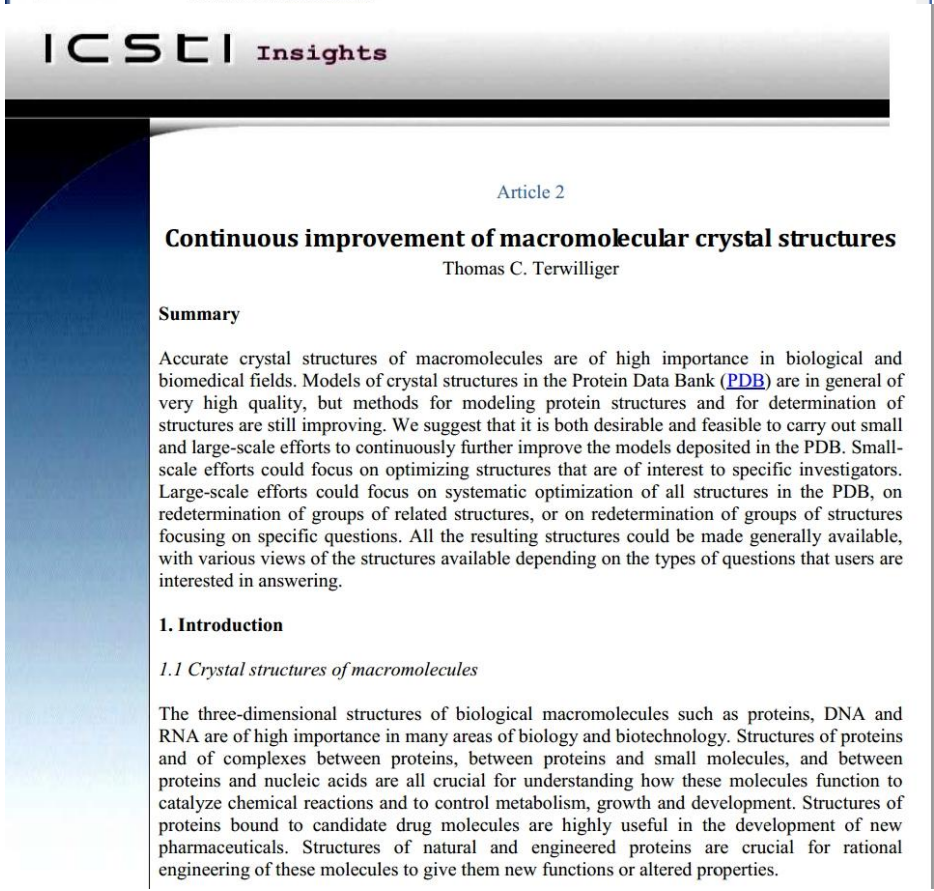


ICSTI Insights

Article 2

Continuous improvement of macromolecular crystal structures

Thomas C. Terwilliger

Summary

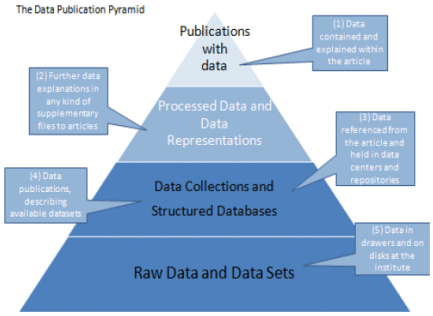
Accurate crystal structures of macromolecules are of high importance in biological and biomedical fields. Models of crystal structures in the Protein Data Bank (PDB) are in general of very high quality, but methods for modeling protein structures and for determination of structures are still improving. We suggest that it is both desirable and feasible to carry out small and large-scale efforts to continuously further improve the models deposited in the PDB. Small-scale efforts could focus on optimizing structures that are of interest to specific investigators. Large-scale efforts could focus on systematic optimization of all structures in the PDB, on redetermination of groups of related structures, or on redetermination of groups of structures focusing on specific questions. All the resulting structures could be made generally available, with various views of the structures available depending on the types of questions that users are interested in answering.

1. Introduction

1.1 Crystal structures of macromolecules

The three-dimensional structures of biological macromolecules such as proteins, DNA and RNA are of high importance in many areas of biology and biotechnology. Structures of proteins and of complexes between proteins, between proteins and small molecules, and between proteins and nucleic acids are all crucial for understanding how these molecules function to catalyze chemical reactions and to control metabolism, growth and development. Structures of proteins bound to candidate drug molecules are highly useful in the development of new pharmaceuticals. Structures of natural and engineered proteins are crucial for rational engineering of these molecules to give them new functions or altered properties.

Raw diffraction images offer the opportunity of:-



- *analysing data at higher resolution than used in the original work*
- *serving as benchmarks in developing improved methods of analysis*
- *checking the interpretation of the symmetries of the crystals*
- *analysing diffraction from multiple lattices present in the crystals*
- *analysing the diffuse scattering that reflects correlated motions or disorder of atoms in the crystals*

Green chemistry: Publications in IUCr Journals

- A total of 137 entries;
- The majority are in Acta Cryst E and thereby Open Access for readers;

Crystallography research example: the platins

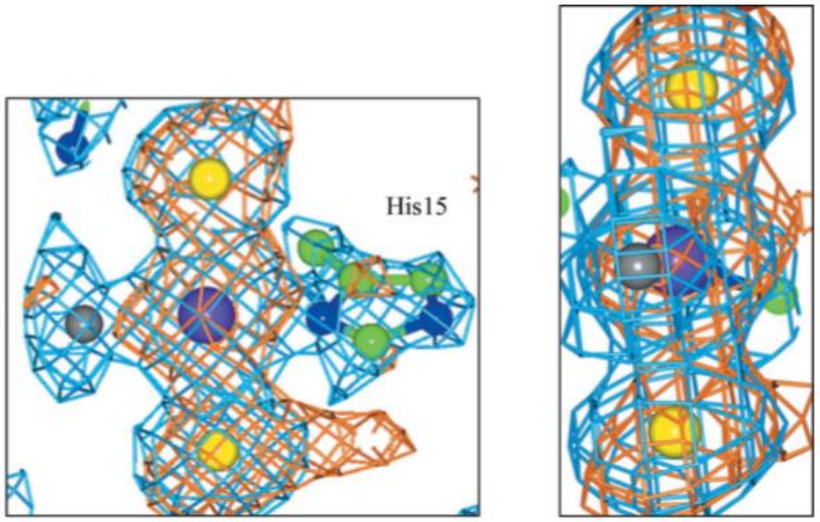


Figure 1
Binding to His15 shows a chemically transformed cisplatin, namely transiodoplatin. (*a*, *b*) The molecule *A* binding site shown in two different views. The $2F_o - F_c$ electron-density map (blue) is contoured at 1.5 r.m.s. and the anomalous difference electron-density map (orange) is contoured at 3σ. The Pt atom is shown in purple, the iodines are in yellow, the chlorine is in grey, C atoms are in green and N atoms are in blue.

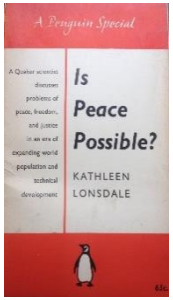
ESRF Medical beamline has conducted Radiation therapy trials on tumours using mice and targeting the Pt K edge.

We are now collaborating to try targeting the iodine K edge as well thus varying the X-ray penetration depth into a tumour.

The hope is to do work with lower quantities of these compounds for a patient.

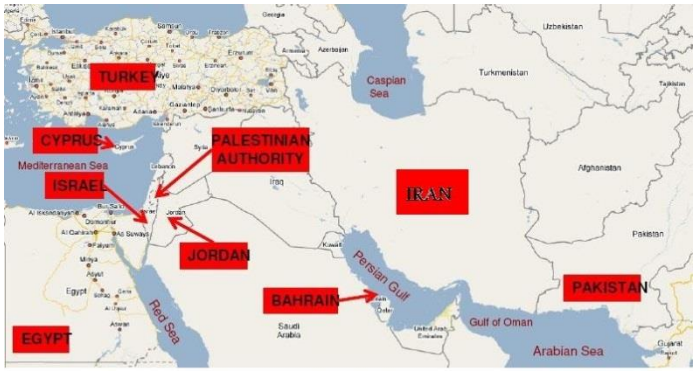
We will soon have made available all the raw data diffraction images of this suite of studies Via the University of Manchester eScholar Repository.

Gold Open Access to the publications, the PDB files and the raw data files.

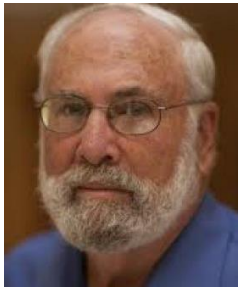


Practical examples of Worldwide capacity building: SESAME synchrotron and peace in the Middle East

- Capacity building; eg ***SESAME*** synchrotron radiation project in Jordan; eg ??an ***African SR project***??



SESAME Members



Dr Hermann Winick
SSRL Stanford

AfLS To be discussed 15-20 November 2015 at ESRF

- One's own Lab: ***multi national research*** staff and students eg in 2011:-

Iraq

Thailand Mexico

Crystallography for the next generation

– RESOLUTION –

issued on the occasion of the IYCr Legacy Conference, Rabat, Morocco, 22-24 April 2015

[…] At a time when scientific endeavour is critical for societal benefit and the importance of crystallography is greater than ever, crystallography remains a science that still has lower visibility than it should,

the IUCr and all partner institutions ***commit***:

- **to enhance the stature of crystallography […]**
- **to build capacity in developing regions of the world […]**
- **to extend further the public understanding of science in general and crystallography in particular […]**

Private endorsement at http://iycr2014.org/into-the-future/conference/resolution

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

Funded under the ICSU Grants Programme 2015

Lead Applicant: International Union of Crystallography
Co-Applicant: European Crystallographic Association

Supporting organizations: UNESCO, ICSU Regional Office for Africa, INDABA, SAASTA

Project plan (2015/2016):

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

+ many additional actions

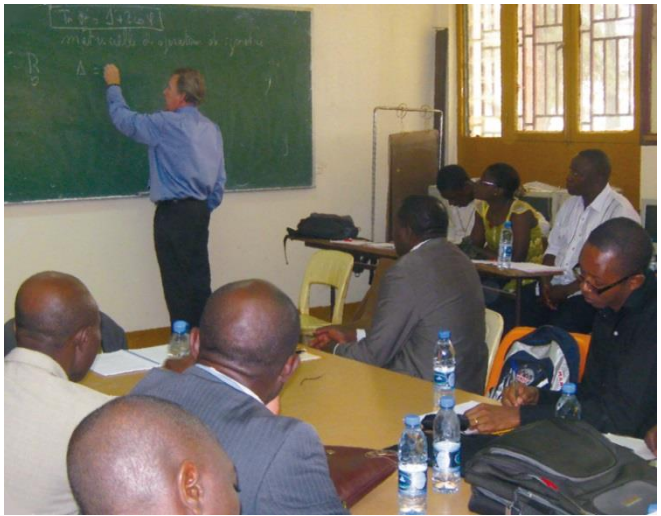
http://www.iycr2014.org/capacity-building/icsu2015

IUCr initiative since 1999

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 (namely, Bruker)



Steering Committee

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IUCr-UNESCO OpenLab IUCr-UNESCO OpenFactory

The **IUCr-UNESCO OpenLab** is a network of operational crystallographic laboratories based in different countries worldwide, mainly in less endowed regions of Africa, South and Central America and South Asia. They are aimed at allowing access to crystallographic knowledge and technology in all parts of the world, key for the fruitful development of science, and to open possibilities for conducting high-level research.

			Dates	Type	Country	Location
2014	1	**Bruker** OpenLab Pakistan	30 Apr 2014 - 8 May 2014	OpenLab Type 2	**Pakistan**	Karachi
	2	**Agilent** OpenLab Argentina	5 May 2014 - 10 May 2014	OpenLab Type 2	**Argentina**	La Plata and Buenos Aires
	3	**Bruker** OpenLab Morocco	20 May 2014 - 20 Jun 2014	Travelling Lab	**Morocco**	Rabat and Agadir
	4	**PANalytical** OpenLab Ghana	9 Jun 2014 - 12 Jun 2014	OpenLab Type 2	**Ghana**	Accra
	5	**Rigaku** OpenLab Cambodia	7 Jul 2014 - 11 Jul 2014	OpenLab Type 2	**Cambodia**	Phnom Penh
	6	**Bruker** OpenLab Uruguay	23 Jul 2014 - 31 Jul 2014	OpenLab Type 1	**Uruguay**	Montevideo
	7	**Bruker** OpenLab Indonesia	18 Aug 2014 - 22 Aug 2014	Travelling Lab	**Indonesia**	Bandung
	8	**Agilent OlexSys** OpenLab Turkey	1 Sep 2014 - 5 Sep 2014	OpenLab Type 2	**Turkey**	Izmir
	9	**STOE DECTRIS Xenocs** OpenFactory	10 Sep 2014 - 19 Sep 2014	OpenFactory	**France and Germany**	Grenoble and Darmstadt
	10	**Rigaku** OpenLab Colombia	27 Oct 2014 - 31 Oct 2014	OpenLab Type 2	**Colombia**	Bucaramanga
	11	**PANalytical** OpenLab Mexico	18 Nov 2014 - 21 Nov 2014	OpenLab Type 2	**Mexico**	Mexico City
	12	**Agilent OlexSys** OpenLab Hong Kong	3 Dec 2014 - 7 Dec 2014	OpenLab Type 2	**Hong Kong**	Hong Kong
	13	**Bruker** OpenLab Vietnam	8 Dec 2014 - 12 Dec 2014	OpenLab Type 2	**Vietnam**	Ho Chi Minh City
2015	14	**PANalytical** OpenLab Turkey	19 Jan 2015 - 22 Jan 2015	OpenLab Type 2	**Turkey**	Ankara
	15	**Bruker** OpenLab Algeria	9 May 2015 - 14 May 2015	OpenLab Type 2	**Algeria**	Constantine
	16	**Bruker** OpenLab Tunisia	14 May 2015 - 23 May 2015	Travelling Lab	**Tunisia**	Monastir and Nabeul
	17	**CCDC** OpenLab Kenya	6 Sep 2014 - 10 Sep 2015	OpenLab Type 2	**Kenya**	Nairobi
	18	**PANalytical** OpenLab Mexico	28 Sept 2015 - 2 Oct 2015	OpenLab Type 2	**Mexico**	Puebla
	19	**Bruker** OpenLab Senegal	5 Oct 2014 - 10 Oct 2015	OpenLab Type 1	**Senegal**	Ziguinchor

Aims and outcomes of the IYCr2014 Summit meetings

The IUCr-UNESCO Summit meetings have been intended to bring together scientists from countries in three widely separated parts of the world, using a common crystallographic theme. There is a real necessity for scientists to think beyond political borders and other distinctions. These meetings, focussed on high level science, also highlighted the difficulties and problems of conducting competitive scientific research in different parts of the developing world.

South-East Asia

Karachi, Pakistan
28-30 April 2014

Summit Declaration

Establishment of the China-Pakistan-India fund

Foundation and 1st meeting of the Pakistani Crystallographic Association Lahore, 9 Oct 2014

1st India-Bangladesh bilateral meeting, Kolkata, 18-19 Sept 2015

New edition of OpenLab planned in Cambodia

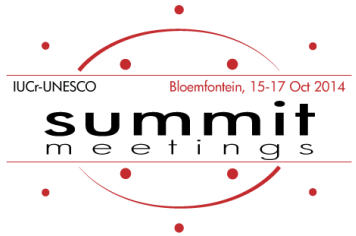
Latin America

Campinas, Brazil
22-24 September 2014

Summit Declaration

Foundation and 1st meeting of LACA, Sao Paulo, 9-11 Sept 2015

New editions of OpenLabs planned in Mexico and Uruguay



Africa

Bloemfontein, South Africa
15-17 October 2014

Summit Declaration

AfCA Steering Committee formed

ICSU proposal approved

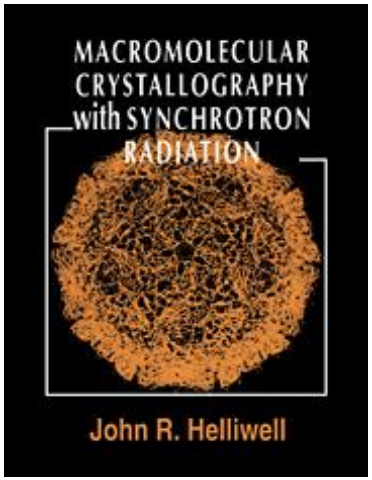
2nd North African Crystallographic Conference, Algeria or Tunisia, mid-2015

1st Crystallographic workshop for Central Africa, Cameroon, Sept 2015

New OpenLabs planned in Senegal, Kenya, Cote d'Ivoire

Acknowledgements

- Wikipedia for their helpful descriptions and quotes from the UN resolutions on global sustainability.
- Michele Zema, Brian McMahon and Peter Strickland of the IUCr Chester, UK for help with slides and detailed comments.
- Dr Cora Lind-Kovacs and Prof Robin Rogers.



Thankyou to the ACA!