

An invitation to support

# IUCr Data Activities 2017

```

#
_audit_conform.dict_name      mmcif_pdbx.dic
_audit_conform.dict_version   4.021
_audit_conform.dict_location
http://mmcif.pdb.org/dictionaries/ascii/mmcif_pdbx.dic
#
loop_
_database_2.database_id
_database_2.database_code
FDB 2FYP
RCSB RCSB036459
#
loop_
_database_PDB_rev.num
_database_FDB_rev.date
_database_PDB_rev.date_original
_database_PDB_rev.mod_type
_database_PDB_rev.replaces
_database_PDB_rev.status
1 2007-01-16 2006-02-07 0 2FYP ?
2 2009-02-24 ? 1 2FYP ?
3 2011-07-13 ? 1 2FYP ?
4 2012-06-13 ? 1 2FYP ?
#
loop_
_database_PDB_rev_record.rev_num
_database_PDB_rev_record.type
_database_PDB_rev_record.details
2 VERSN ?
3 VERSN ?
4 JRNL ?
#
_pdbx_database_related.db_name      TargetDB
_pdbx_database_related.db_id       RVO884c
_pdbx_database_related.details
_pdbx_database_related.content_type unspecified
#

```

Please support

IUCr Data

Activities 2017



We invite past and prospective sponsors to support the crystallographic information and data-related activities planned by IUCr working groups during 2017. We realise that, in an IUCr Congress year, you will have many such requests to consider; but we hope that you will look favourably on this one, given the importance of the work we are doing to improve the handling of scientific data in our field, and the productivity and success of our previous workshops and symposia.



**James R. Hester**

Chair, IUCr Committee for the Maintenance of the CIF Standard



**John R. Helliwell**

Chair, IUCr Diffraction Data Deposition Working Group

# Main activities for 2017

## **DDDWG Workshop: Research Data Management**

**ACA Meeting, New Orleans, LA, USA**

**26 May 2017**

The crystallographic community prides itself on its archiving of processed diffraction data and associated derived atomic coordinates. The natural extension is to extend this to primary (*i.e.* raw) diffraction data. This workshop at the 2017 Annual Meeting of the American Crystallographic Association focusses on the practical issues of securing raw diffraction data preservation. It addresses two main aspects:

What every experimentalist needs to know about recording essential metadata of primary diffraction data. This will include sample preparation and characterization; correct recording of instrument axes, correction factors, calibration, instrument manufacturers; attention to diffuse scattering or other interesting “metadata”.

Research Data Management policy mandates and requirements on Principal Investigators (PIs). This will include metadata standardization, data repositories, and primary data linking to publications.

## **COMCIFS Dictionary Writing Workshop**

**IUCr Congress, Hyderabad, India**

**21 August 2017**

The Dictionary Writing Workshop will provide participants with the skills to create high-quality dictionary definitions and complete data dictionaries suitable either for inclusion within the CIF/mmCIF framework or as standalone dictionaries for use within other data frameworks, such as NeXus. Participants will be guided during practical sessions towards the goal of producing a complete dictionary or set of additional definitions in a scientific domain of interest to them.

# Other activities in 2017

Members of DDDWG and COMCIFS will take part in or contribute to a number of other activities during the 2017 IUCr Congress programme:

**Keynote Lecture:** The Science is in the Data

John R. Helliwell

24 August 2017

**Microsymposium:** Scientific value of raw data

Chairs: Brian McMahon, Loes Kroon-Batenburg

24 August 2017

**Microsymposium:** Crystallographic data and structure validation from data collection to publication – IUCr setting standards

Chairs: Alexander J. Blake, Zbigniew Dauter

27 August 2017

**Microsymposium:** Robust programming for CIF, NeXus, and related file structures

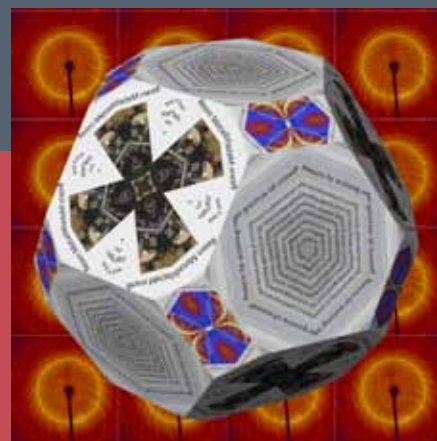
Chairs: Herbert Bernstein, John Bollinger

27 August 2017

## Future directions

### IUCr Committee on Data

At the General Assembly of the IUCr in Hyderabad in August 2017, the Diffraction Data Deposition Working Group will be transformed and subsumed into a new standing committee on data. This new body will advise the IUCr Executive Committee on all aspects of data with respect to policy and actions to be taken. It will have a formal relationship with COMCIFS, which will continue with its technical brief to manage the CIF standard. This represents the IUCr's strong commitment to continue to extend and develop best practice in data management and quality.



## Past activities

### COMCIFS

#### Workshop: Crystallographic Information and Data Management

A Satellite Workshop to the 28th European Crystallographic Meeting

University of Warwick, Coventry, UK

<http://www.iucr.org/resources/cif/comcifs/workshop-2013>

#### Symposium: Crystallographic Information and Data Management

A Satellite Symposium to the 28th European Crystallographic Meeting

University of Warwick, Coventry, UK

<http://www.iucr.org/resources/cif/comcifs/symposium-2013>

### DDDWG

#### Workshop; Diffraction Data Deposition

A Satellite Workshop to the 27th European Crystallographic Meeting

University of Bergen, Bergen, Norway

<http://www.iucr.org/resources/data/dddwg/bergen-workshop>

#### Workshop; Metadata for raw data from X-ray diffraction and other structural techniques

A Satellite Workshop to the 29th European Crystallographic Meeting

Rovinj, Croatia

<http://www.iucr.org/resources/data/dddwg/rovinj-workshop>



## Recent publications

### COMCIFS

Hall, S. R. & McMahon, B. (2016). The Implementation and Evolution of STAR/CIF Ontologies: Interoperability and Preservation of Structured Data. *Data Science Journal*, **15**, p.3.

Bernstein, H. J., Bollinger, J. C., Brown, I. D., Grazulis, S., Hester, J. R., McMahon, B., Spadaccini, N., Westbrook, J. D. & Westrip, S. P. (2016). Specification of the Crystallographic Information File format, version 2.0. *J. Appl. Cryst.* **49**, 277–284.

Bollinger, J. C. (2016). A portable general-purpose application programming interface for CIF 2.0. *J. Appl. Cryst.* **49**, 285–291.

Hester, J. (2016). A Robust, Format-Agnostic Scientific Data Transfer Framework. *Data Science Journal*, **15**, p. 12.

### DDDWG

Terwilliger, T. (2014). Archiving raw crystallographic data. *Acta Cryst.* **D70**, 2500–2501.

Kroon-Batenburg, L. M. J. & Helliwell, J. R. (2014). Experiences with making diffraction image data available: what metadata do we need to archive? *Acta Cryst.* **D70**, 2502–2509.

Meyer, G. R., Aragão, D. *et al.* (2014). Operation of the Australian Store.Synchrotron for macromolecular crystallography. *Acta Cryst.* **D70**, 2510–2519.

Guss, J. M. & McMahon, B. (2014). How to make deposition of images a reality. *Acta Cryst.* **D70**, 2520–2532.

Terwilliger, T. & Bricogne, G. (2014). Continuous mutual improvement of macromolecular structure models in the PDB and of X-ray crystallographic software: the dual role of deposited experimental data. *Acta Cryst.* **D70**, 2533–2543.

Kroon-Batenburg, L. M. J., Helliwell, J. R., McMahon, B. & Terwilliger, T. C. (2017). Raw diffraction data preservation and reuse: overview, update on practicalities and metadata requirements. *IUCrJ* **4**, 87–99.

# How can you support?

## 1. Financial contributions

Although the IUCr provides significant travel, accommodation and administrative support, external funding also helps to provide travel support for participants who would not normally attend a parent crystallographic meeting (thereby allowing us to broaden the variety of input to these events). It also contributes towards venue hire and allows recording of some events, useful documentation for workshop participants (detailed programmes, article reprints, background and briefing notes), and scope for open-access publication of derivative papers.

We invite supporters to consider contributions of

(a) **GBP 400** towards either of the main workshops to be held in 2017 (*i.e.* the DDDWG Data Management Workshop in New Orleans or the COMCIFS Dictionary Workshop in Hyderabad); or

(b) **GBP 600** to be used to provide support as needed at either or both of the workshops and any additional activities that come under the purview of COMCIFS, DDDWG or the IUCr Committee on Data.

# What will you get out of it?

In response to direct financial or in-kind contributions, we shall display your company or organization logo in all publicity and documentation material relating to the event supported (web pages, programme books, introductory and acknowledgement slides). We shall acknowledge sponsors in official workshop reports.

If you take advantage of option (b) to support all our activities during the year, we shall also display your logo and acknowledge your support in the "Other activities" listed on p. 4, and, during 2017, we shall display your logo on the IUCr Commission on Data web page.

We also expect that direct collaboration or contribution to public discussion will enhance the community's appreciation of your active interest in an increasingly important element of best scientific practice.



## 2. In-kind contributions

Direct financial contributions are not always possible from academic institutions, not-for-profit organizations or publicly funded service providers. However, we are very willing to advertise in-kind support from institutions or organizations that cover the travel, accommodation and registration costs of speakers, tutors or workshop organizers.

## 3. Community engagement

We consider the active engagement of companies, scientific or data organizations and service providers to be at least as important in supporting our aims and activities. We encourage you to participate by sending delegates to our varied events, by contributing to public discussion forums, joining in standardization efforts, co-authoring scholarly articles, etc. We value your support not only in funding our work, but also in becoming active partners in our goal to increase the value of scientific data in the structural sciences.



### Web links

#### **IUCr Committee on Data**

<http://www.iucr.org/iucr/governance/advisory-committees/committee-on-data>

#### **DDDWG**

<http://www.iucr.org/resources/data/dddwg>

#### **COMCIFS**

<http://www.iucr.org/resources/cif/comcifs>

#### **Public forum for input on diffraction data deposition**

<http://forums.iucr.org/viewforum.php?f=21>

For more information, please contact

#### **Brian McMahon**

International Union of Crystallography  
5 Abbey Square  
Chester CH1 2HU  
UK

[bm@iucr.org](mailto:bm@iucr.org)

+44 (1244) 342878

# Thank you!

Thank you for considering this invitation,  
and for your interest in and commitment  
to the IUCr's initiatives on data.

Previous supporters include

**DECTRIS**<sup>®</sup>

**IUCr Journals**  
CRYSTALLOGRAPHY  
JOURNALS ONLINE



**THE CAMBRIDGE  
CRYSTALLOGRAPHIC  
DATA CENTRE**



FIZ Karlsruhe  
**ICSD**

**OxfordCryosystems**

**WILEY**



**Rigaku**

**CRYSTAL  
IMPACT**

**ACS**  
Chemistry for Life<sup>®</sup>



**RSC** | Advancing the  
Chemical Sciences

**D | C | C**

**LIBRARY  
HSILIRB**

WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

**THE UNIVERSITY OF WESTERN AUSTRALIA**  
Advancing International Frontiers

