

J R Helliwell and B McMahon report on the Data aspects of the BCA CCG with RSC Autumn 1 day meeting

“Communicating Crystallography”

Organised by Peter Wood (CCDC) & Simon Coles (National Crystallography Service, University of Southampton).

Deputy Chair & Chair of the CCG

This was a very interesting conference on the topic “*Communicating Crystallography*” featuring publications, data and use of the www (see Appendix 1 details of the programme). We each made active contributions BMcM a presentation and JRH as a Panellist including a very short formal presentation (see Appendix 2). There were approximately 50 participants. One of the participants was deaf and the whole meeting was recorded by two stenographers working alternately through the day.

In the Panel discussion some of the points that arose were:-

- (a) What exactly is metadata?
- (b) The null results of crystallisation experiments ie that fail to produce crystals are very valuable, so might these ‘raw data’ in future be recorded somehow eg at IUCr Journals?
- (c) Raw diffraction data is a blurred topic in that in the electronic detector ‘counting chain’ the X-ray measured photons undergo various corrections and even pixel resolution manipulation.

Regarding point (a) the IUCr Diffraction Data Deposition Working Group (DDDWG; see <http://forums.iucr.org/viewtopic.php?f=21&t=343> for their recent triennial report) have proposed and had accepted by the IUCr Executive Committee to have a 1 day workshop on the *Metadata of raw data* prior to the ECM 29 in Rovinj, Croatia. The opening speaker Dr Loes Kroon-Batenburg of the University of Utrecht, a very active member of the IUCr DDDWG, has accepted our invitation to speak and lead the discussion. Dr Simon Coles has also agreed to speak.

Point (b) we believe can usefully be discussed within the DDDWG albeit outside our explicit terms of reference. A possible proposal would be to concatenate this with the ‘difficult data sets’ new article category proposed for J Appl Cryst by L K-B.

Point (c) is also a good one and indeed as, for example, more is understood about diffuse, non-Bragg scattering, detector counting chain optimisations to better measure both Bragg and non-Bragg scattering might be made (such as expand the dynamic range of the detector and/or better preserved raw diffracton data).

Simon Coles stressed the aspect emphasised by BMcM in his talk that the halving of Acta Cryst E articles are a genuine loss to the open scientific literature of the new science that they communicated and their excellent processed and derived data quality as it seems that these articles are no longer getting published.

Appendix 1

http://ccg.crystallography.org.uk/documents/AM_2014_programme.pdf

Chemical Crystallography Group Autumn Meeting 2014 Wednesday 19th November 2014

Venue: RSC Chemistry Centre, Burlington House, London .

10:30 Registration (COFFEE/TEA)

Session 1 – Crystallography in Education (Chair: Simon Coles)

“Communicating Crystallography”

11:00 Dr Anna Warren (Diamond Light Source)

“Diffracting your expertise onto the next generation – crystallography outreach”

11:30 Dr Peter Hoare (University of Newcastle)

“Development of bite-sized chemistry teaching & learning resources utilising a free subset of the Cambridge Structural Database”

12:00 Prof Chick Wilson (University of Bath)

“Frontiers of crystallography: a research-led learning experience”

12:30 LUNCH

Session 2 – Publishing and Crystallography (Chair: Pete Wood)

14:00 Dr Guy Jones (RSC)

“Publishing chemical crystallography in high impact journals”

14:30 Dr Serin Dabb (RSC)

“The National Chemical Database Service and our vision for a community data repository”

14:45 David Sait (RSC)

“Social media at Education in Chemistry”

15:15 COFFEE/TEA

Session 3 – Disseminating Structures (Chair: Lynne Thomas)

15:45 Brian McMahon (IUCr)

“From structural data to structural knowledge”

16:15 Panel discussion session, including **Serin Dabb** (RSC), **Ian Bruno** (CCDC), **Simon Coles** (NCS) & **John Helliwell** (University of Manchester & IUCr DDDWG) as panel members, on the topic of: “Data, databases & deposition”

17.15 CLOSE

This meeting has been kindly sponsored by Agilent

Appendix 2

JRH's, by necessity, short presentation at the start of the Panel session was the short summary of the IUCr DDDWG presented by him to the IUCr General Assembly in Montreal. Slide snapshots are provided here:-



CONGRÈS ET ASSEMBLÉE GÉNÉRALE
DE L'UNION INTERNATIONALE DE CRISTALLOGRAPHIE

Diffraction Data Deposition Working Group (DDDWG) report to the IUCr General Assembly Montreal

John R Helliwell on behalf of the
DDDWG

CONGRESS AND GENERAL ASSEMBLY
OF THE INTERNATIONAL UNION OF CRYSTALLOGRAPHY



Recommendations from the DDDWG for the upcoming Triennium

- IUCr Commissions to define their metadata;
- *J. Appl. Cryst.* to introduce a 'Difficult Raw Data' Section (Loes Kroon-Batenburg);
- A centralised crystallographic repository of raw data set metadata should be scoped, inc a search interface, leading to a pilot service;
- With a viable pilot metadata registry **authors should** provide a permanent and prominent link from an article to their raw data sets underpinning a journal publication.

Issues for the IUCr

- The IUCr's science involves 'Big data up towards the level of the data-deluge of the Square Kilometre Array radio telescope; we may have to consider subsets of data retention or limited time periods for retention;
- Rights of access to publicly funded, but unpublished, crystallographic research data after *e.g.* 3 to 5 years.

Members of the DDDWG

- *John R Helliwell and Brian McMahon (UK),* Chair and Co-Chair;
- *Steve Androulakis (Australia)*
- *Sol Gruner (USA)*
- *Loes Kroon-Batenburg (Netherlands)*
- *Tom Terwilliger (USA)*
- *John Westbrook (USA)*
- *Heinz-Josef Weyer (Switzerland)*