

**32nd European
Crystallographic Meeting**

ECM 32 ♦ Vienna Austria ♦ 18. – 23. 08. 2019



IUCr's Committee on Data Workshop

“Data Science Skills in Publishing: for authors, editors and referees”

Organizers:

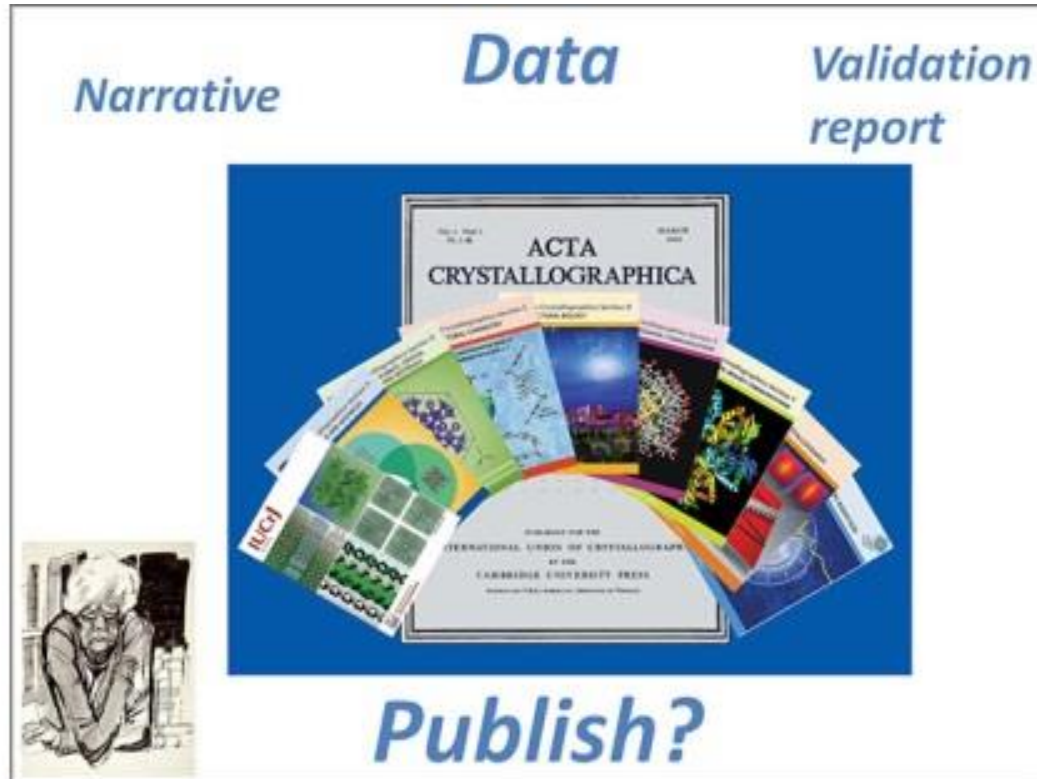
John Helliwell (University of Manchester, UK)

Brian McMahon (IUCr, R&D Department, UK)

Date: 18th August 2019

Time: 8:25 a.m. to 5 p.m

Introduction



The Editor as Gatekeeper>>>



Is refereeing the data as well sustainable?



"The old pearly gates looked nice, but they were hell to maintain."

Also the need for consistency; the crystallographic information file and Check cif>>>

*But, can Validation Reports cover everything that needs to be checked?
No, you need to check all three:-*

Narrative

Data

*Validation
report*

Narrative

Data

*Validation
report*

*IUCr chemistry journals have followed
this **exemplary practice** and are an
inspiration to other fields of
crystallography to follow their lead*

*Dr Madeleine Helliwell
Acta Cryst C Coeditor*



*As EinC IUCr Journals
(1996-2005) I could see
Madeleine's Acta Cryst C
editorial work on the
submissions by authors*

*In the mid 2000s with IUCr Chester we surveyed this topic and also considered archiving **and use of raw diffraction data** [1].*

At that time harnessing raw data archiving was a gleam in the eye!

[1] Strickland, P., McMahon, B. & Helliwell, J. R. (2008). Integrating research articles and supporting data in crystallography. *Learned Publishing*, **21**, 63-72.

Right, let's go to it

- Sunday 18th August 2019 proposed programme:
Session 1 Chair: Annalisa Guerri
Morning: 08:25 - 12:00
08:25-08:30 John R Helliwell: "Introduction to the Workshop"
08:30-09:00 Tony Linden: "Data refereeing and editing in chemical crystallography; the Acta Cryst C experience"
09:00-09:30 Brian McMahon: "The vital role of Crystallographic Information Files in chemical and biological crystallography to underpin the databases' validation reports"
09:30-10:00 Ton Spek: "Platon and raw diffraction data opportunities for chemical crystallography publishing"

10:00-10:30 *** COFFEE ***
Session 2 Chair: Brian McMahon
10:30-11:00 Miguel Aranda: "The role of raw powder diffraction data in peer review; past, present and future"
11:00-11:30 Kay Diederichs and Manfred Weiss: "Diffraction data deposition and publication"
11:30-12:00 Loes Kroon-Batenburg: "Raw data opportunities for biological crystallography publishing"
12:00-13:00 *** Lunch ***
Afternoon: 13:00 – 16:00
Session 3 Chair: Simon Coles
13:00-13:30 Simon Coles, Suzanna Ward and Carl Schwalbe: "Correcting the public record of chemical crystallography science"
13:30-14:00 Mariusz Jaskolski: "Correcting the public record of biological crystallography science"
14:00-14:30 Petra Bombicz: "Overview of the role of data reviews and tutorial reviews in improving crystallographic science training"

14:30-14:45 *** Comfort break ***

Session 4 Chair: Brian McMahon
14:45-15:15 Simon Billinge: "Moving towards a more data-centric scientific literature"
15:15-15:45 Gillian Holmes: "IUCrData - update on data publication and practices at the IUCr"
15:45-16:00 John R Helliwell: "Overview of the new opportunities in and a harmonisation of peer review of "data with validation report with article narrative" practices"

16:00-16:30 *** General Discussion ***

16:30-17:00 === TEA ===
18:00 Opening Ceremony of ECM32