Poster

Raw Data Letters - describing and publishing raw diffraction data in a FAIR way

Simon Coles, John Helliwell, James Hester, Loes Kroon-Batenburg

University of Southampton

s.j.coles@soton.ac.uk

IUCrData, the peer-reviewed open-access data publication from the International Union of Crystallography (IUCr), has launched a new section: Raw Data Letters as a collaborative innovation of IUCr Journals with the IUCr Committee on Data.

Future raw data sets will become increasingly large and no one group will be able to analyse all the scientific content in a timely manner and others will need access to raw crystallographic datasets for open-science-based research to proceed at a rapid pace. Further, there is an increasing need to better support validation of results in a more in-depth and transparent way for anyone wishing to reuse them. However, credit should be attributed fairly among experiment designers, data collectors and those who subsequently use the data to establish new results.

The new section publishes short descriptions of crystallographic raw data sets from X-ray, neutron or electron diffraction experiments, in the biological, chemical, materials science or physics fields, and provide a persistent link to the location of the raw data. Raw Data Letters can support different goals through making raw data available e.g.:

- Describing interesting features in raw data sets, allowing researchers to attract attention to aspects that could be of interest to methods and software developers or may be relevant to the structural interpretation,
- The structure could have been solved and published elsewhere, but the letter describes interesting features that were observed but ignored in the original determination,
- The letter could describe remarkable features, but not attempt to interpret them; in this way the data attract attention and the original authors get credit for their work,
- The raw data show Bragg reflections to a reasonable resolution but the structure could not be solved, enabling attempts by others but
  for the data generators to get credit for their work,
- Letters might describe the reuse of publicly available data by improved methods.

Submissions are now being welcomed and Notes for authors and submission instructions are available from the IUCrData website. This is early days for the Raw Data Letters section, so working with our Co-editors (https://iucrdata.iucr.org/x/services/editors.html) to develop and facilitate publication of your data is welcomed.