

## The birth of *IUCrData*

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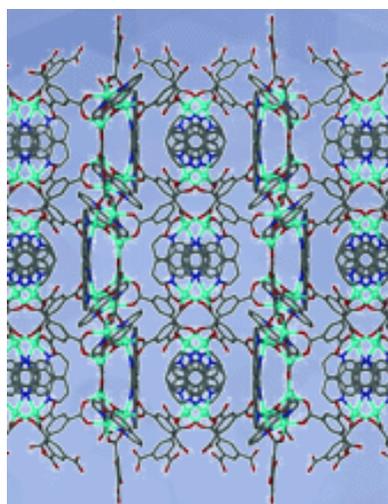
The International Union of Crystallography is delighted to announce the launch of a new open-access data publication, *IUCrData*. This innovative publication aims to provide short descriptions of crystallographic datasets and datasets from related scientific disciplines.

The first phase of this venture will provide a new home for the *Data Reports* previously published in *Acta Crystallographica Section E: Crystallographic Communications*. The *Data Reports* will provide authors with a vehicle to publish brief, peer-reviewed reports on individual crystal structures with a rapid publication turnaround and the ready availability of results guaranteed by an open-access publication. Individual data articles will be deliberately short and to the point. They will provide a mechanism to rapidly publish structures that might otherwise not be available to the scientific community, as well as ensuring that peer-reviewed information on uniquely determined structures is readily accessible. In the new data publication, reports of previously published structures will be considered when clear differences in data quality, consideration of packing or different data-collection conditions, such as temperature or radiation source, are involved.

To ensure continuity in the transitional phase, the current Main Editors of *Acta Crystallographica Section E* will also serve as Main Editors on *IUCrData*, along with former *Acta E* Main Editor, Jim Simpson. We are pleased that 19 current and recently retired Co-editors of *Acta E* have agreed to join the editorial team, bringing a wealth of experience to *IUCrData*.

*Data Reports* in *IUCrData* will comprise the following components:

- (i) A one or two sentence *Synopsis*.
- (ii) A short *Abstract* (100–150 words).
- (iii) A *Structure description* section (CIF dataname `_publ_manuscript_text`) containing comments about the structure. Overlap between this section and the *Abstract* will be kept to a minimum. Together they will include: a brief description of the molecule with salient features; a brief summary of the packing features; a related structure or structures for comparison; and a short statement of the relevance of the molecule and/or chemical background to the study.
- (iv) A chemical scheme and an *ORTEP*-style plot of the molecular structure (a polyhedral plot for inorganic compounds).
- (v) If packing features are discussed, a packing plot together with a hydrogen-bond table.
- (vi) A packing plot for all polymeric compounds (coordination polymers and inorganics).
- (vii) A synthesis and crystallization section.
- (viii) Tabular structural data.
- (viii) References – these will be kept to a minimum and, in particular, self-referrals will be kept to an absolute minimum.
- (ix) A refinement section will only be needed if there are unusual features to the refinement, such as disorder, use of SQUEEZE or omission of reflections.



A key characteristic of the new *Data Reports* will be the brevity of the discussion. The metric data and plots will appear in the main body of the publication and will provide the bulk of the information. Readers will be able to access to the complete diffraction data, the submitted CIF and the full checking output.

*Data Reports* are easy to prepare using the IUCr's *pubCIF* software which can be downloaded free of charge from <http://pubcif.iucr.org>. To submit to *IUCrData*, simply upload

your CIF file (processed and validated with *pubCIF* and containing the text and the structural data) together with the structure factors (if not embedded in the CIF) and graphics files in the usual way *via* the *IUCrData* website: <http://iucrdata.iucr.org/x/services/submit.html>.

We are grateful to all who have contributed to the successful birth of this latest addition to the IUCr family of publications. We look forward to the growth of *IUCrData* and to a successful first year of publication in 2016!