

Reporting 3D ED structures made easier: the changes in the core CIF dictionary to allow consistent, correct, and complete reporting of 3D ED structure refinements

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3D electron diffraction (3D ED, also known as MicroED) has become a viable and increasingly popular method for solving and refining crystal structures. As the number of solved and published structures grew, it became quickly clear that, on top of the scientific challenges related to the method, the community has one more problem to solve – the consistent reporting of the structure analyses.

The crystallographic science immensely profits from the existence of the Crystallographic Information Framework (CIF, [1,2]), of which the central element is the definition and use of the Crystallographic Information File (also CIF, or CIF file). Essentially all published crystal structures are made available in this format, making them easily accessible by other researchers, databases, and crystallographic software.

The basis of the CIF files is the dictionary that defines valid entries and their syntax. The main CIF dictionary (called the core CIF dictionary) was designed before the advent of the 3D ED methods, and, therefore, it was not adapted to describe structures refined against 3D ED data. To address this problem, a committee was established within the Horizon2020 ITN project NanED, with the aim of proposing an update to the CIF dictionary that would allow a better incorporation of the 3D ED structures in the CIF. The committee worked in close collaboration with the IUCr officials, especially Brian McMahon. After the first draft of the proposal, there have been several rounds of discussions and updates. The final discussion took place in a dedicated Discord discussion group and was open to every interested person from the crystallographic community.

The result was a proposal for an update of the core CIF dictionary that has already been approved by the IUCr Committee for the Maintenance of the CIF standard (COMCIFS). At the web address https://www.iucr.org/resources/cif/dictionaries/cif_core, the current development version is already available, and the new CIF entries will be part of the next official release of the core CIF.

The new items can be roughly divided into three categories:

- terms of general relevance that were generalized to include 3D ED, for example, the new option to specify that absolute structure was determined using dynamical diffraction effects, entries allowing to specify the fluence and dose received by the crystal, or entries for the specification of crystal mosaicity
- terms specific to 3D ED, but applicable in general to 3D ED data, for example, the specification of the use of precession electron diffraction, illumination mode (SAED vs. micro/nanobeam), specification of the level of diffraction theory used, or the new entries allowing to specify the difference electrostatic potential values
- terms specific for dynamical refinement from 3D ED data. This approach does not have an equivalent in the X-ray structure refinement, and thus several new terms had to be introduced, e.g., the specification of the refined crystal thickness, the treatment of the crystal shape in the refinement, or the z-score value for the determination of absolute structure.

The presentation will introduce the upgrade, discuss the critical aspects of the proposed changes, and outline some guidelines for the practical application of the new terms.

[1] *International Tables for Crystallography Volume G: Definition and exchange of crystallographic data*, edited by S. R. Hall and B. McMahon, International Union of Crystallography (2006).

[2] Bernstein, H. J., Bollinger, J. C., Brown, I. D., Gražulis, S., Hester, J. R., McMahon, B., Spadaccini, N., Westbrook, J. D. & Westrip, S. P. (2016). *J. Appl. Cryst.* **49**, 277-284.

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