Poster

A toolkit for young crystallographers in need of more learning resources

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The Cambridge Structural Database (CSD) [1], the crystallographic database for organic and metal-organic molecules, now contains over 1.25 million crystal structures. This wealth of data makes it an invaluable resource both in research and in education, both in crystallography and chemistry as well as other subjects.

In this poster, we will focus on resources and activities from the Cambridge Crystallographic Data Centre (CCDC), the curators of the CSD, and from collaborators in the community to support young crystallographers and educators in their learning journey.

One of the essential tools for a crystallographer is the CIF file. Despite this, reading and writing a CIF is not always an easy task as it presents a complex syntax; moreover, it is often generated automatically by refinement software, making the crystallographer less in need to directly edit it. We will thus present our *Short Guide to CIFs* [2], an introductory handout to CIF syntax designed for crystallographers who wishes to gain more confidence in reading CIFs and editing them.

As crystallography has many challenging topics, we will then present *DECOR*, the Database of Educational Crystallographic Online Resources [3]. This project was started by Prof Zdilla at Temple University and has been hosted on the CCDC website since 2020. *DECOR* is a collection of teaching resources shared by educators in the community for other educators and students to use in their teaching and learning. Resources cover a variety of topics, including crystal lattices, symmetry, diffraction, disorder, twinning, and are in a range of formats, from slides to videos, from practical exercises to interactive webpages. Presenting different approaches and formats for the same topic allows to accommodate for different learning preferences.

Another challenge that students and educators face is the relative scarcity of raw diffraction images available for teaching. This is even more impactful when diffractometers are not available or are difficult to access. In these regards, we will present a new resource created from the collaboration between researchers at Newcastle and the CCDC, Diamond Light Source, Bruker, Rigaku and STOE: *RODIN*, a Resource Of Diffraction Images, Newcastle [4]. This collection of raw data, accessible from *DECOR*, complements the CSD Teaching Subset [5], and is designed and available for teaching, training and demonstration.

[1] Groom, C. R., Bruno, I. J., Lightfoot, M. P., Ward, S. C. (2016). *Acta Cryst.* **B72**, 171-179. DOI: *10.1107/S2052520616003954*.

[2] A Short Guide to CIFs. *https://www.ccdc.cam.ac.uk/community/access-deposit-structures/deposit-a-structure/guide-to-CIFs/*.

[3] DECOR, the Database of Educational Crystallographic Online Resources.

https://www.ccdc.cam.ac.uk/community/education-and-outreach/education/decor/.

[4] Waddell, P. G., Michael R. Probert, M. R., Johnson, N. T. *RODIN (Resource of Diffraction Images, Newcastle): Raw diffraction data for teaching, training and demonstration*, in preparation.

[5] Battle, G. M., Allen, F. H., Ferrence, G. M. (2010). *J. Chem. Ed.* **87(8)**, 809-812. DOI: *10.1021/ed100256k*.