Oral presentation

RODIN: a resource of diffraction data for teaching, training and demonstration

Natalie T. Johnson [1], Michael R. Probert [2], Paul G. Waddell [2]

[1] *The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, CB2 1EZ, UK*
[2] *School of Natural and Environmental Chemistry, Newcastle University, Newcastle upon Tyne NE1 7RU, UK*
paul.waddell@ncl.ac.uk

When it comes to teaching crystallography, at most stages of education the start and end points are covered. Crystal growing experiments are synonymous with elementary and high school science and the Cambridge Structural Database (CSD) teaching subset [1] exposes students to the 3D structures of chemicals in the form of crystal structure determinations. Little attention has been given to the steps taken between crystal and structure, steps that require access to the raw diffraction data. Compared to the almost 1.3 million structures available in the CSD there is a dearth of diffraction images available for teaching purposes.

To redress the balance, in collaboration with the CCDC, Diamond Light Source, Bruker, Rigaku and STOE, we have created a resource of raw diffraction data specifically curated to extend the remit of the CSD Teaching Subset and make diffraction images available for teaching, training and demonstration. These data are available online through DECOR [2].

To compile this resource a range of compounds represented in the CSD Teaching Subset, with which educators and students may already be familiar, were chosen in addition to some new entries with the aim of representing a broad range of chemical disciplines. Examples of experiments collected at different wavelengths, using different collection strategies and a variable temperature study are also included. Data are available from a range of different instruments including examples collected at a synchrotron.

Complete with access to DIALS [3] and links to other data processing software packages, it is hoped that this collection will be a good starting point for a larger resource. We actively encourage others to contribute more datasets to expand the range of crystallographic experiments available. In addition, we plan to develop specific teaching exercises that will use the raw datasets and hope that users are also inspired to create and share their own.

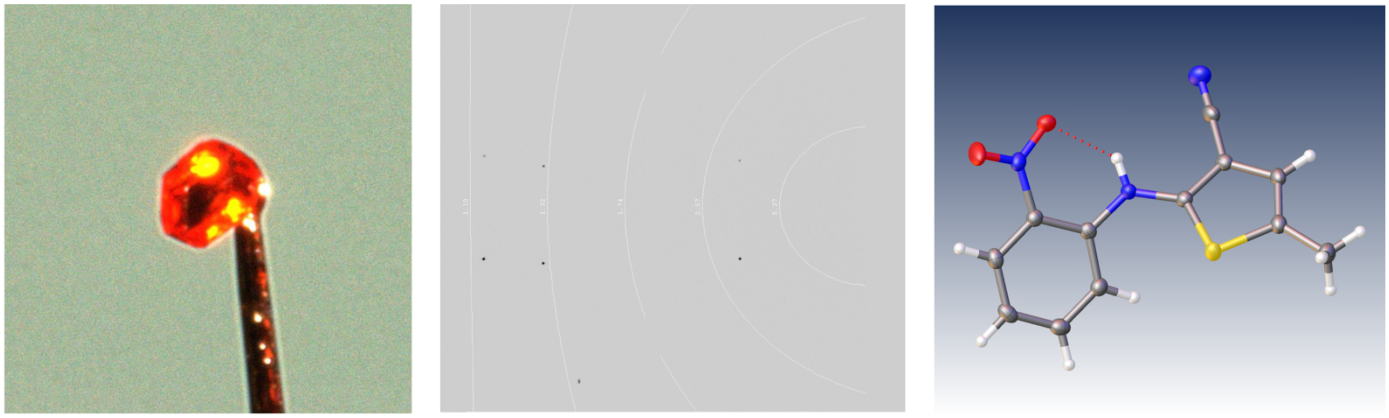

Figure 1. A crystal of 5-methyl-2-((2-nitrophenyl)amino)-3-thiophenecarbonitrile (left) and the corresponding crystal structure (right). The steps between the two rely on the diffraction images (centre)

[1] Battle, G. M.; Allen, F. H. (2010). J. Chem. Ed. 87(8), 809-812.

[2] DECOR, https://www.ccdc.cam.ac.uk/community/education-and-outreach/education/decor/ (accessed 2024/04/04).

[3] Winter, G.; Waterman, D. G.; Parkhurst, J. M.; Brewster, A. S.; Gildea, R. J.; Gerstel, M.; Fuentes-Montero, L.; Vollmar, M.; Michels-Clark, T.; Young, I. D.; Sauter, N. K.; Evans, G. (2018). Acta Cryst. D74, 85-97.