Oral presentation

Using Crystal Structures from the Cambridge Structural Database in Schools

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The Cambridge Structural Database (CSD) [1] is the crystallographic database for organic and metal-organic molecules and it contains over 1.25 million crystal structures. In this session we will explore how teachers can leverage the database and associated software for teaching STEM subjects in schools, highlighting free tools and resources.

First of all, educators and students can freely access the structures in the database online from any device using Access Structures [2]. The webpage for the structure selected provides some basic information about it and an interactive 3D visualiser where the molecules and the structure can be observed in detail. Students can moreover retrieve geometric information independently by measuring bonds, angles and torsions.

We will then present the CSD Teaching Subset [3], which aims at helping teachers with the task of selecting from 1.25 million structures in the database the most suitable and interesting for their students. The CSD Teaching Subset is indeed a collection of over 850 structures from the CSD specifically selected with educators from the community to be of particular interest in the teaching of crystallography and chemistry. The CSD Teaching Subset is accessible online and it also comes pre-installed with the free version of Mercury [4]. Mercury is the visualisation software for small molecules from the CCDC; its free version includes features for visualisation and basic analysis that enable educators and students to gain a deeper understanding of concepts studied in the classroom.

We will also share case studies and examples of resources that demonstrate the use of crystal structures for teaching in schools for different age groups, such as the teaching modules and educational videos, and materials created in the community with the support of the CCDC Engagement Grants.

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

[2] Access Structures: https://www.ccdc.cam.ac.uk/structures/?

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

[4] Free Mercury: https://www.ccdc.cam.ac.uk/solutions/software/free-mercury/