

MS48 What should undergraduate students learn about crystallography?

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Using crystallographic databases in undergraduate education – the example of the Cambridge Structural Database

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Abstract

Crystallography underpins and informs lots of different subjects, such as chemistry and biology, and fields, from pharmaceutical to agrochemical, from energy storage to the food industry. It is not a surprise then how extensively crystallographic data can be used in education.

In this talk we will focus on what undergraduate students can learn from crystallographic databases, taking the Cambridge Structural Database (CSD) and the associated software, the CSD Software as a case study.

First, we will present the CSD Teaching Subset and relevant teaching material, and how it can be used for teaching in combination with WebCSD and our visualization software Mercury. The CSD Teaching Subset is a collection of over 750 structures selected by the CCDC in collaboration with educators in the community, free for download and use in education. The structures in the CSD Teaching Subset are particularly good to demonstrate and exemplify a range of topics, from isomerism to chirality, from VSEPR theory to symmetry operations, from molecular interactions to reaction mechanisms. One of the strong suits that make using the CSD in education an asset is the possibility to visualise molecules and structures in 3D in Mercury. Indeed, being able to explain a three-dimensional concept in a 3D space rather than on a 2D board is considered of crucial importance by educators in the communities who shared their experiences with us.

Another great advantage of using crystal structures in teaching is to provide real examples and case studies, thus connecting theory to scientific challenges.

There is even more that undergraduates can learn from crystallographic databases and from the crystallographic community. Indeed, the crystallographic community is regarded as an example to follow for the way they format their data using the CIF file and how data are shared and maintained in databases such as the CSD. Using more advanced functionality from the CSD Software, students can learn how to search a database with over 1.1 million structures. This is per se a gateway for students to develop and improve a range of skills: from performing a literature review to good data sharing practices, and learning not only how to answer a research question, but also how to interrogate the data.

There is a lot that undergraduates can learn from crystallography and the crystallographic community and we believe that the use of crystallographic databases like the CSD can support them and enhance their learning.

References

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