

structure determination, and despite its involvement in 25 Nobel Prize awards, crystallography is poorly represented in University teaching curricula; at best, it is simply noted at high school level. As a consequence, there is sometimes a limited understanding of crystallographic results, e.g. some medicinal chemists regard all conformational information as being tainted by crystal packing forces, precision indicators are misunderstood, and so on. One way of improving this situation is to promote the use of crystal structures in high school and undergraduate teaching. By taking crystallography to its beneficiary subjects in an educational way, we may hope to generate a greater familiarity with the results and a deeper interest in the experimental aspects of the technique.

The Cambridge Structural Database (CSD) contains a wealth of chemical information, and a subset of around 500 entries is freely available for teaching purposes at http://www.ccdc.cam.ac.uk/free_services/teaching/ [1]. Chemistry is a 3D subject, too often introduced and taught using 2D and 2.5D representations. However, the fully interactive exploration of crystal structures (e.g. via JMOL or Mercury) provides fundamental understanding at both school and undergraduate level, making students think and learn in 3D. Comparing the conformations of ethane and *n*-butane, studying chirality in L- and D-alanine, or exploring important structure types such as alkaloids, steroids, and metal-organics with various coordination geometries, brings chemistry to life. The teaching area of the CCDC website also contains a series of modules that use both the subset and the complete CSD to address specific chemical topics [2]. These include (teaching subset): aromaticity, rings strain and conformation, valence shell electron pair repulsion, and hapticity, as well as (full CSD): mean molecular dimensions, halonium ions as reaction intermediates, metal-carbonyl back bonding, and geometrical interconversions in four-coordinate metal complexes. This set of modules is now being extended to include, among others, studies of reaction pathways and studies of hydrogen bonding and other intermolecular interactions.

[1] G.M. Battle, F.H. Allen, G.M. Ferrence, *J.Chem.Educ.* **2010**, *87*, 809-812 and *87*, 813-818. [2] G.M. Battle, G.M. Ferrence, F.H. Allen, *J.Appl.Cryst.* **2010**, *43*, 1208-1223.

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Experimental determination of chemical structure in the undergraduate curriculum

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Exercises in experimental structural chemistry have been introduced into the first and second-year chemistry laboratory at Otterbein University. In the first-year laboratory, student groups were assigned one of twelve amino acids. Students researched crystallization methods using the web-based Cambridge Structural Database (WebCSD) and grew crystals for X-ray analysis. Selected crystal samples were analyzed using the Bruker SMART X2S diffractometer. Using the Mercury software package, students analyzed molecular geometry, hydrogen bonding, unit cells, density and crystal packing. This activity serves as an integrated exercise to teach and reinforce concepts of chemical bonding, molecular structure, intermolecular forces and the nature of crystalline materials. In the second-year inorganic chemistry laboratory, students used X-ray diffraction as a significant tool for structural characterization of products from a multi-week independent synthesis project.

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Writing crystal structure reports in collaboration with undergraduate students

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An approach for increasing the impact of undergraduate scientific training with chemical crystallography through a laboratory report writing exercise has been developed. In an introductory chemistry curriculum, one of the first things we teach our students is the structure of atoms and molecules in order to help them develop a “molecular understanding”. With drawings or models, students learn to answer questions such as, “What is the angle between these three atoms?” or “What is the shape of this molecule?” In organic chemistry, students are then introduced to chirality and stereochemistry. With modern instrumentation, molecular structures, and often the absolute structure of resolved compounds, may be experimentally determined in a matter of hours, adding another means to depict realistic molecules for students that also links learning to the experimental laboratory. The speed and ease of use of such instrumentation today is exceptional, such that it may be introduced more widely to undergraduate students in coursework, even when there is limited time available for a crystallography module.

As scientific educators, it is also important to mentor students in the communication of new knowledge. Just as chemical crystallography can be a fast, effective tool to experimentally observe the structure of molecules and enhance student learning of structure, it can also provide an inspiring opportunity for students to write short, scientific journal style reports that may be edited and published in collaboration with a crystallographer. This contribution will focus on a course module used to expose undergraduate students to small molecule crystallography, and in particular to the preparation of the resulting crystal structures for publication. With examples of both published and unpublished structures, topics will include: compound choice, structure validation, literature and database searching, and the writing of descriptions of crystal and molecular structures, absolute structure, packing and intermolecular interactions.

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“Applied crystal chemistry” for chemists and materials scientists

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The contribution describes a 30-year experience of teaching a general course in solid-state chemistry for undergraduates, which introduces at the same time the main concepts of crystallography, gives an introduction into structure analysis techniques and makes links to the courses in inorganic chemistry, organic chemistry, and biochemistry. Such a combination can be beneficial for bringing the fundamental crystallography (basics and techniques) closer to its “users” – chemists, materials scientists, biologists, and can be considered as an attempt of a course in “applied crystallography”. The aim of the course is to teach chemists, which chemical information can be retrieved from a crystal structure, and how. This is complementary to more generally