

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/](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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### MS.83.3

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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

accepted courses, which teach how to obtain structural information and to describe crystal structures. In the presentation we demonstrate several examples from lectures and practicals.

[1] E.V. Boldyreva, *J. Appl. Cryst.* **2010**, *43*, 1172-1180.

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### Measures of complexity

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The term *complex* is frequently attributed to crystal structures with giant unit cells containing hundreds or thousands of atoms. It is commonly used in a non-defined, fuzzy way. It would be advantageous, however, to have a quantitative measure of structural complexity, to be able to compare periodic and quasiperiodic structures, for instance. Why could this be of interest? Some physical properties, which strongly depend on medium- and long-range order, could be related to complexity and used as knowledge basis for their prediction. Another interesting question is the time evolution of a structure (crystal growth) as function of its complexity. For instance, it is obvious that a crystal with a simple cubic close packed structure such as copper will have a much simpler growth mechanism than a ternary quasicrystal.

Recently, it was suggested in different context to apply the concept of *algorithmic complexity* to crystal structures, periodic and quasiperiodic ones [1]. This way of quantifying the complexity of a system is related to the minimum size of an algorithm needed for its full description. If we apply this concept to the Fibonacci sequence (FS) in the  $nD$  description, for instance, then we obtain the same algorithmic complexity for the quasiperiodic FS and all its periodic approximants, from the smallest to the largest one. This is somehow counterintuitive.

If we use the concept of *symbolic complexity*, we arrive at drastically different results for periodic and quasiperiodic structures. Symbolic complexity is related to the number of different structure motifs (AET) as a function of system size, which is a function of the repeat period in case of the approximants and of the system size in case of the FS. For another example, let's start from a simple periodic structure and apply a sinusoidal incommensurate modulation. This immediately increases the period of the incommensurately modulated structure (IMS) to infinity. However, the algorithmic complexity of the IMS is only slightly higher than that of the small-unit-cell periodic structure. In case of a commensurate modulation, we can continuously increase the number of atoms per supercell without changing the algorithmic complexity of the structure, while the symbolic complexity would grow with the system size to infinity.

Another kind of complexity measure is the *combinatorial complexity*, which can best account for high symmetries of structural subunits (clusters). The less probable (symmetric) a configuration is the higher is its complexity. For instance, in case of equally sized hard spheres, close sphere packings such as the *cF4*-Cu structure are more probable from different point of views than the *cP1*-Po structure. Consequently, the latter has the higher combinatorial, but lower algorithmic complexity, and both have equal symbolic complexities.

In conclusion, no single complexity concept alone is able to reflect all facets of structural complexity, to quantify what we intuitively grasp.

[1] E. Estevez-Rams, R. González-Férez, *Z. Kristallogr.* **2009**, *224*, 179-184.

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## MS.84.2

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### Frustrated Order

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Frustration occurs whenever a local order (atomic configuration) cannot be extended perfectly throughout the space. A paradigmatic example is that of polytetrahedral order encountered in dense packing models. In that case, a direct connection with icosahedral order is present, which makes the frustration concept useful in different contexts, like clusters, glassy materials or quasicrystals. Similar situations can be found with covalent materials and soft matter systems; in most cases, the real structure shows intricate relations between ordered regions and topological defects[1].

We shall first recall how frustration and order interfere in the general case. Then, some new results will be presented, related to dense frustrated order in confined (cylindrical) geometry, a topic which might prove interesting in the nanophysics context. Indeed, a rich phase diagram is found, with many different types of different order occurring while increasing the cylindrical radius, showing a nice competition between chiral, icosahedral, crystalline and disclinated icosahedral order.

[1] J-F-Sadoc et R. Mosseri, “*Geometrical Frustration*”, Cambridge University Press, **1999**.

**Keywords:** frustration, defects, nanostructures

## MS.84.3

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### Local Rules and Global Order

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An appropriate concept for describing an arbitrary discrete atomic structure is the *Delone set* (or an  $(r;R)$ -system). Structures with long-range order such as crystals involves a concept of the space group as well.

A mathematical model of an *ideal monocrystalline matter* is defined now as a Delone set which is invariant with respect to some space group. One should emphasize that under this definition the well-known periodicity of crystal in all 3 dimensions is not an additional requirement. By the celebrated Schoenflies-Bieberbach theorem, *any space group contains a translational subgroup with a finite index*.

Thus, a mathematical model of an ideal crystal uses two concepts: a Delone set (which is *of local character*) and a space group (which is *of global character*).

Since the crystallization is a process which results from mutual interaction of just nearby atoms, it is believed (L. Pauling, R. Feynmann et al) that the long-range order of atomic structures of crystals (and quasi-crystals too) comes out local rules restricting the arrangement of nearby atoms.

However, before 1970's there were no whatever rigorous results until Delone and his students initiated developing the *local theory of crystals*. The main aim of this theory was (and is) *rigorous derivation* of space group symmetry of a crystalline structure from the pair-wise identity of local arrangements around each atoms. To some extent, it is analogous to that as, in due time, it was rigorously proved that space group symmetry implies a translational symmetry.

In the talk it is supposed to expose some results on local rules for