MS46-O5 An Enhanced Hirshfeld Test - Validating Atomic Vibrations in Crystal Structures

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The current routine procedure for publishing crystal structures of small molecules includes structure validation via the the IUCr CheckCIF service. [1] Part of that procedure is the Hirshfeld test [2] which ensures that the atomic vibrations, encoded as Atomic Displacement Parameters (ADPs), are physically reasonable. While the Hirshfeld test is fast and efficient at finding potential problems in the structural model, there exist a number of borderline cases where the test is not able to find implausible ADPs. In other cases the CheckCIF routine might raise alerts where the structure is actually perfectly fine.

An improved procedure will be presented which aims to address these problems. The procedure is based on the Hirshfeld test and inspired by the 'RIGU' restraint from the Shelxl [3] program. This is achieved by analyzing the ADPs characteristics in all three spacial dimensions instead of only validating its expansion in bond direction and taking the atomic masses applied to a harmonic oscillator model into account.

This procedure achieves its goal of finding problematic ADPs in cases that are not found by the traditional Hirshfeld test and is able to reasonably evaluate the ADPs of atoms with significantly different atomic masses e.g. carbon – hydrogen bonds in neutron diffraction studies.

[1] Spek *Acta Cryst (2015).* C71, 9-18.

[2] Rosenfield et al., Acta Cryst (1978). A34, 828–829.

[3] Thorn et al., *Acta Cryst.* (2012). A68, 448-451.

Keywords: Validation, ADPs

MS47 Teaching & Education

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MS47-O1 It is never too early, or too late to start

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Education tends to become more and more narrow. Knowledge about the world around and inside is being segmented into an ever-growing number of fields and sub-fields: mathematics, physics, chemistry, biology, planetary sciences, geology, mineralogy, and the list goes on. Not only are the humanities, sciences and arts taught separately, but there is also a growing trend not to teach all of these subjects to the same child. Instead, education is restricted to a narrow focus from an early age, limiting the breadth of skills and interests of any individual. As a result of this education technique, people tend to lose a general view of the world as a whole. Not only is this destructive for the individual, but places great limits on the development of society and culture.

Crystallography is a unique and fascinatingly multidisciplinary field that offers numerous links between the arts and sciences, between maths and chemistry, biology and physics. The objects of crystallography are beautiful, its language is strict and logical, yet open to intuition, and its applications are variable. Crystallography is, in some respects, a “meta-science”, affording those that study it an integrated, harmonious vision of nature. As such, crystallography is an excellent subject to pursue for life-long education, and an exemplary discipline around which to focus public engagement efforts in both the sciences and arts.

In the present contribution we suggest a concept of using crystallography as a tool for a wholesome, balanced education that starts with children aged 3-6 years old and ends with seniors. At no point is a background in the sciences assumed. Some aspects of this concept have already been successfully tested in Novosibirsk, Russia, and in Edinburgh, UK. Others are yet to be implemented; we welcome volunteers to join us in this educational experiment. In particular, we discuss examples of communicating science to kids, of using crystallographic texts during French and English lessons. We also emphasise the co-teaching of crystallography and art, where the principles of each discipline are mutually reinforced. Hands-on sessions, drawing, and crystal growing can be ideally combined with the solving of mathematical problems, performing chemical and physical experiments, exploring natural objects (minerals, plants, food), and the discussion of modern materials and devices. Educational formats depend on the target audience and desired outcome.

Figure 1. Tiling - an art or science?

Keywords: public engagement, school education, multi-disciplinary teaching

MS47-O2 A cross-field perspective on Symmetry & Crystal to introduce Crystallography

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Crystallography uses two important tools, a concrete object: crystal, and an abstract description: symmetry. To illustrate the science of crystallography to the public, examples using the symmetry and crystal will be illustrated.

Symmetry as proportion and light played an important role in aesthetics (symmetry means "right measures / proportions" in Greek). Vitruvius developed the virtues of proportion and symmetry in architecture and in nature, as shown by Leonardo da Vinci in its “human body” drawing. Architecture makes extensive use of symmetry: symmetry is present in Islamic mosques, Chinese pagodas, Hindu temples and Gothic cathedrals. Tiling patterns are also a great example of symmetry, as shown in Islamic cultures in the Middle Ages.

Crystals shapes and facets comply geometric rules. Studying their symmetries allows us to differentiate the crystals. In the 19th century German and French researchers developed symmetry to classify all the crystals. They introduce the concepts of lattice, axis, center, and mirror plane of symmetry. Crystallographers have given a new meaning to the word symmetry itself, which had hitherto been reserved for architectural purposes. This classification of crystals according to their symmetry and lattice structure is still with us today. The symmetry links the shape of the crystals to their atomic structure and it is important for studying the physical properties of crystals. This abstract relationship between crystal and symmetry was confirmed in 1912, together with the periodicity of the crystal, by the first X-ray diffraction experiments.

We can use the crystal and the symmetry to focus public interest on crystallography and to show children and students the importance of observations, models and representations in scientific approaches. As an illustration, we will present several workshops using the facilities of Physiquarium and KaleidoLab. The capacity of KaleidoLab to generate models is used for the creation of "on-live" wallpapers and videos.

This presentation is the result of different actions: Voyage dans le Cristal exhibition (*) Krystallopolis website (**) and KaleidoLab workshop (***) and we thank colleagues who contributed to these actions, Marc DeBoissieu, Dominique Cornuejols, Thibaut David, Yannick Lacaze, René Guinebretière.

* http://www.iycr2014.org/resource-materials/voyage

** http://www.krystallopolis.fr/

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http://neel.cnrs.fr/IMG/KaleidoLab_Symetrie-cest-quoi_14dec15-ss-sc