Ducks in space groups!

Students grasping 3D-arrangement of symmetry elements with hands-on models

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Symmetry considerations are vital in chemistry and even more so in crystallography [1-2]. Typically, students first come into contact with this during their studies in the context of stereochemistry or spectroscopy where usually the Schönflies notation is used. Learning and teaching about molecular symmetry naturally requires spatial imagination. To develop and refine this, models and model kits are of outmost importance and are readily available for a broad range of purposes [3].

The description of crystalline matter from a crystallographer's point of view naturally requires translational symmetry to be considered. Therefore, the applied framework to learn and discuss about molecular symmetry needs to be extended, also leading to the introduction of the Herman-Mauguin notation. From our teaching experience this transition and especially the introduction of translational symmetry components is difficult and something students struggle with. These difficulties typically culminate when it comes to the combination of symmetry elements and their assembly to give space groups. The connotation in the International Tables for Crystallography, section A [4] is not particularly intuitive to understand and to apply without the help of models.

We herein present large scale (i. e. typically 50 x 50 x 50 cm), physical 3D models of complete space groups (Figure 1) to promote student's spatial imagination and to help understanding the construction of space groups by symmetry elements. The models were designed and built to fulfil three basic requirements: (1) to be accurate space group representations containing the symmetry symbols, (2) to visually resemble the conventional 2D space group notation if viewed along the respective crystallographic axis and, (3) to allow students to assemble asymmetric units within the unit cell by themselves.

Grabbing fosters grasping!

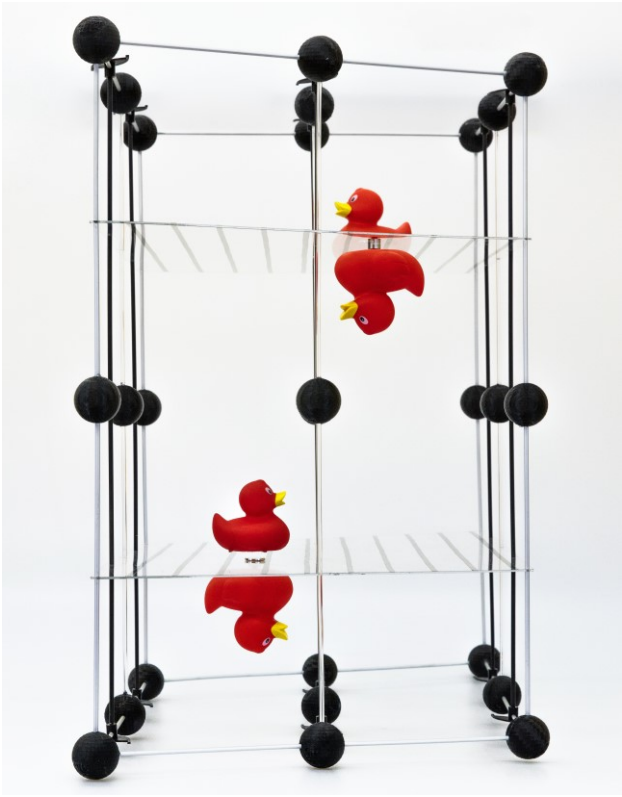

Figure 1. Model of space group $P2_1/c$ along the crystallographic *c* axis. The rubber ducks represent asymmetric unit's content.

[1] Jaffé, H. H. (2013). *Symmetry in Chemistry;* New York: Dover Publications.

[2] Glasser, L. (1967). *J. Chem. Educ.* **44**, 502.

[3] Flint, E. B. (2011). *J. Chem. Educ.* **88**, 907–909.

[4] Brock, C. P.; Hahn, T.; Wondratschek, H.; Müller, U.; Shmueli, U.; Prince, E.; Authier, A.; Kopský, V.; Litvin, D. B.; Arnold, E.; Himmel, D. M.; Rossmann, M. G.; Hall, S.; McMahon, B.; Aroyo, M. I. (2016). *International tables for crystallography*, Sixth edition A; International Union of Crystallography: Chester, England.

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