Oral presentation

Can you still get "Marshed"? – Experience *versus* algorithms

C. W. Lehmann

Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr, Germany

lehmann@kofo.mpg.de

In this day and age single crystal small molecule crystallography has become a household technique in most chemistry departments and crystal structure databases like the CSD reflect this development through a nearly exponential growth of new entries . Several factors have contributed to this increase: better instrumentation, faster and more powerful computers and user friendly software. Especially the latter had a huge impact with regard to the number of people determining their own crystal structures. Once the domain of highly specialized scientists, sometimes guarding their knowledge secretively, terms like orientation matrix, start phases, E-values or block-diagonal-refinement have all but disappeared from the vocabulary of people entering the field.

Instead state-of-the-art software includes pre-determined workflows ranging from setting up data collections to fully automated structure solution and refinement, sometimes within a few minutes from mounting the crystal onto the diffractometer. With such prospects advertised by the manufacturers of diffraction systems it is not surprising that more and more users of such highly automated processes no longer feel the need to obtain fundamental crystallographic training. A development that starts early on during academic education in chemistry, as degree curricula contain only the most basic crystallographic concepts.

A not uncommon attitude towards this lack of formal crystallographic knowledge emphasizes that you can drive a car without knowing anything about the internal combustion engine and more and more people determining crystal structures expect the same of the diffraction equipment. The possible pitfalls are manifold. There are unit cells either too small or with an apparently too high symmetry, because weak reflections have been overlooked. This problem then progresses via incomplete data sets and might or might not be spotted during space group determination. Again missing knowledge about systematic extinctions and weak statistics leads to wrong space groups [1], whereby the forced presence or absence of inversion symmetry leads to the wrong chemical interpretation of disorder. Repeating the refinement in a non-centrosymmetric space group might be the answer, provided the correct transformation matrix is applied. And of course the opposite holds true as well, if large correlations between parameters are spotted and treated correctly. Damping is rarely the answer. This list can be expanded a lot further.

What remedies are there? Foremost good basic training! And if the degree course doesn't offer this, then attending one or more of the excellent summer schools should be mandatory for every user of diffraction systems. As an alternative experts still around should make use of the modern tools for online teaching. Short video sequences explaining the do's and don'ts can help a lot to spread crystallographic knowledge. Not being shy and asking a colleague, who has many years of experience will also help to avoid basic mistakes. This holds in particular if alerts generated by the excellent algorithms behind the software carrying out crystallographic plausibility checks are taken seriously, before the manuscripts are submitted. Anonymised examples from my own laboratory and from refereeing will be given to illustrate the above made case.

[1] Henling, L. M., Marsh, R. E. (2014). *Acta Cryst.* C**70**, 834.