

FORTY YEARS OF MARSHING: IS THE MISSED SYMMETRY PROBLEM NOW SOLVED? A.L.Spek, Utrecht University, Padualaan 8, 3584CH Utrecht, The Netherlands. a.l.spek@uu.nl

The assignment of the proper space group to a crystal structure, i.e. the one that uniquely describes its symmetry, is not always trivial. Real world issues such as disorder, twinning and pseudo-symmetry may blur the way to a unique assignment with X-Ray diffraction techniques. Often one has to settle with the best approximation given the data and the purpose of the study.

For various reasons, structure analysts do not always report their structures with the best symmetry description. That may lead to false claims of supposedly interesting chemistry that in hindsight are purely based on refinement artefacts.

In the late 1970ies, Dick Marsh together with Verner Schomaker and others started to investigate and report on this type of problems in reported structures in published papers. Early papers had titles such as ‘Some Incorrect Space groups in Inorg. Chem., Volume 16’.

Over time, Dick published numerous similar corrections. Others picked up this type of investigations as well. Not everybody was happy when their name featured in papers of ‘Marshed’ structures. A very relevant issue is that context is that the underlying experimental data (e.g. reflection data and images) are not always available. Those primary data are definitely needed for a proper ‘verdict’.

Dick did his explorations by flipping through journal issues, looking for suspect ORTEP illustrations and special relation between atoms in ‘independent’ molecules. Nowadays, in combination with the archived data in the CSD, easy to use tools are available to spot routinely structures with possibly missed symmetry.

Issues like missed symmetry led eventually to the idea to routinely check structure reports prior to publication. The IUCr introduced the checkCIF facility for that purpose.

One would assume that, given the readily available tools, missed symmetry and Marshded structures are no longer an issue. For that reason, all structures entered in the CSD during the 5 years 2013-2017 were inspected with the ADDSYM tool in PLATON. The result of that analysis will be shown.