Invited Lecture

Space groups – unnecessary knowledge from yesterday?

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In the past, structure solution was unthinkable without profound expertise in space groups. One had to determine the Laue class given by the symmetry of the diffraction pattern and then to check the systematic absences. This led to one or more possible space groups and the structure solution needed to be tested in these space groups. Later programs like *XPREP* [1] facilitated the determination of the space group. Possible systematic absences were automatically tested and criteria like R_{int} of the appropriate Laue class or the numbers of entries in the CCDC [2] were combined to a figure of merit (CFOM), which helped to decide which space group should be tested first. Then George Sheldrick wrote the program *SHELXT* [3], which solves the structure in space group *P*1 and only the information of the correct Laue class is necessary as input. After solving the structure, the space group and the atom type of each found atom are determined. *SHELXT* works very well for small molecules and even the assignment of the atom types most frequently is correct. This has opened the way to an automated structure and refinement process delivered by the diffractometer manufacturers and also the step- by-step refinement often needs only a few clicks and even inexperienced users can solve and refine simple structures very quickly without deep knowledge of space groups.

However, there are structures that cannot be solved by *SHELXT* like very large structures, structures with pseudo-symmetry or high amount of disorder or derived from twinned crystals etc. Then programs like *SHELXD* [4] are necessary and these programs need the correct space group. In such problematic cases, even *XPREP* sometimes fails or the output needs some more human interpretation. Some examples will be shown.

Recently, false statements about a ‘new’ structure could be found although there is an identical structure known in a different space group setting or for the ‘new’ determination a wrong space group was used [5, 6].

The answer to the question raised in the title is therefore clearly **no**.

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[4] Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112.

[5] Herbst-Irmer, R. & Stalke, D. (2024). *Angew. Chem. Int. Ed.* e202319571.

[6] Cicirello, G., Wang, M., Sam, Q. P., Hart, J. L., Williams, N. L., Yin, H., Cha, J. J. & Wang, J. (2023). *J. Am. Chem. Soc.,* **145**, 8218.