

s3.m1.o5 **Twinning in Chemical Crystallography: How to Discover what is Disguised.** M. Bolte, *Institut für Organische Chemie, J.-W.-Goethe-Universität, Marie-Curie-Str. 11, 60439 Frankfurt/Main, Germany, E-mail: bolte@chemie.uni-frankfurt.de*

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Twinning is a crystal growth anomaly in which the specimen is composed of separate domains whose orientations differ in a specific way. This leads to an overlap of the reciprocal lattices of the different components, which complicates the structure determination, because one has to find out the geometrical relationship of the twin components, which is in other words the twin law.

In certain cases the overlapping reciprocal lattices might veil the correct unit cell and simulate a pattern of higher symmetry (Fig. 1). As a result of that, the crystallographer is faced with two problems: recognizing the twinning and finding the correct cell.

The use of area detectors is a great deal of help in these cases, because the complete reciprocal space has been recorded and not only some points in space. Thus, even after removing the crystal from the diffractometer, the complete data is available for examination.

With the aid of a non-merohedral twin¹ as an example it will be demonstrated how to recognize a twinned crystal structure, discover the correct unit cell and finally refine² the structure in a satisfactory way. The advantages of disposing of area-detector data will be emphasized.

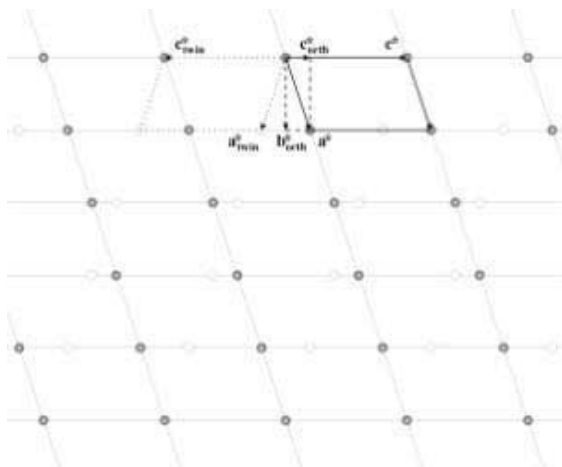


Fig.1. Section of the reciprocal space displaying the relation of the twinned monoclinic cell with the simulated orthorhombic cell.

[1] Hensen K, Faber A. & Bolte M. "trans-Tetrabromobis(3,5-dimethylpyridine)-germanium(IV), a non-merohedral twin", *Acta Crystallogr. C.*, (1999), C55: 1774 - 1775.

[2] Sheldrick, G.M. "SHELXL-97- Program for the refinement of crystal structures", (1997), University of Göttingen, Germany.