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# Symmetry Relationships between Crystal Structures. Second edition. By Ulrich Müller and Gemma de la Flor. IUCr/Oxford Science Publications, 2024. Pp. XVIII + 368. Price GBP 55.00. ISBN 978-0-19-285832-0

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The first edition of this textbook was written by Ulrich Müller, with a paperback edition published in 2017, where a few typos I had mentioned in my review (Nespolo, 2013) were corrected. In this new edition (retaining the subtitle *Applications of Crystallographic Group Theory in Crystal Chemistry*), a new chapter (Chapter 24) covers the Bilbao Crystallographic Server and other relevant computer programs. Several topics have been extended, for example, the "treatment of equivalent description of crystal structures and chirality" is now presented in a dedicated chapter (Chapter 9), whereas it was previously included in the chapter on conjugate subgroups and normalizers of space groups. References have also been updated. Most of the *Appendices* in the first edition now have the status of a full chapter, in a new Part III, whose main content is the new chapter on the *Bilbao Crystallographic Server*. Here I concentrate of the changes/updates and I refer the reader to my review in 2013 for more details on the core content of this textbook.

In the first edition, a section (3.3) was devoted to the *Application of (n+1)×(n+1) matrices*, which is now part of the previous section on *Affine mappings*. Far from being just a cosmetic change, this modification anticipates the much larger use of the 4 × 4 matrices throughout the text, now largely preferred to the matrix-column presentation: a commendable choice which makes the formulas more explicit and easier to understand for beginners and readers less used to the (**W**,**w**) formalism. There is also a new, albeit brief, section (7.4.1) devoted to sectional layer groups and penetration rod groups, the diperiodic and monoperiodic, respectively, equivalents of site-symmetry groups of non-periodic objects. This is a hot topic today, due to the increasing technological interest for subperiodic modules building up new materials; unfortunately, the lack of crystallographic education often leads to weird and physically meaningless expressions like 2D-materials, 1D-materials, and even 0D-materials (Nespolo, 2019).

Another short new section (13.4) is devoted to *Wrong settings of space groups*, with examples of perovskite structures and how tricky can be the choice of the correct space group when going down a symmetry path.

Section 16.7 on *The role of non-realizable intermediate groups in a Bärnighausen tree* is another most welcome addition. Here we learn about the transition path from a centrosymmetric supergroup to two possible chiral subgroups between which one finds a Sohncke achiral group where the atomic equilibrium positions still fulfil the full symmetry of the centrosymmetric supergroup. An intermediate structure would realize the breaking of the inversion symmetry only through anharmonic atomic displacement parameters, leading to twinned domains differing only for the handedness of their thermal motion – something very hard to confirm experimentally.

The last addition to this new edition is Chapter 24, devoted to the *Bilbao Crystallographic Server*. There are several publications (a full list is available on the server website) that present the server and its routines, along with a wiki containing tutorials and a large collection of presentations and solved exercises from schools organized by the Commission on Mathematical and Theoretical Crystallography. However, this chapter serves more as a step-by-step guide to using the server in practice, providing a welcome landing point for readers who have worked through the preceding theoretical chapters. Although far from being a complete instruction manual, which would span a full book

and is difficult to conceive, considering that the server is constantly evolving, it provides newcomers with adequate information to begin their exploration of the server.

I am particularly happy to see that most of the (small) imperfections I had mentioned in my review of the first edition have been addressed; however, there are a couple of exceptions.

Page 74: it is still not explained why $\overline{6}$ is used instead of 3/*m*, something that a beginner may have some difficulties grasping, especially since what is observed in the morphology is indeed 3/*m*. This is the reason why in old classifications crystal classes corresponding to point groups of type $\overline{6}$ and $\overline{6}2m$ were placed in the trigonal instead of the hexagonal system (von Groth, 1895).

Page 248: the widespread, yet imprecise expression 'merohedral twin' is still used instead of the more precise 'merohedric twin'. Regrettable.

Overall, there is no doubt that this is one of the most complete and important textbooks on crystallography in the XXI century and stands out against a plethora of less rigorous books that should never have been published. The moderate price is a further incentive to obtain a personal copy to keep handy for one's daily crystallographic tasks.

Last but not least, one should point out the existence of a German version of this second edition (Müller, 2023), which also has a new Chapter 24 *Unterstützende Rechenprogramme* (supporting computer programs). It deals with the Bilbao Crystallographic Server and the IUCr Symmetry Database (which is only marginally mentioned in the second English edition). In this German editon, chapter 24 at just six pages is therefore much less detailed than the equivalent chapter in the English second edition (19 pages). A Spanish version of the first edition (Müller, 2013) also exists.

## References


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