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book reviews

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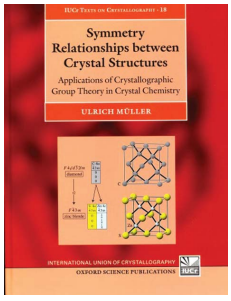

Symmetry Relationships between Crystal Structures. By Ulrich Müller. IUCr/Oxford Science Publications, 2013. Pp. XVI + 332. Price (hardcover) GBP 49.95. ISBN 978-0-19-966995-0.

Symmetry Relationships between Crystal Structures – which brings the subtitle *Applications of Crystallographic Group Theory in Crystal Chemistry* – is a much awaited text (also available in German and Spanish) summarizing the method developed by Hartmut Bärnighausen to derive hettotypes from known aristotypes, or *vice versa* to build possible aristotypes from known hettotypes, *via* group–subgroup relations which consider the whole structural data: space groups, site-symmetry groups of the occupied Wyckoff positions, changes in these groups as well as splitting of the positions when going down an aristotype–hettotype relation. The book has had quite a long gestation, passing through lecture notes prepared by the author for various schools organized in several countries which partly served as a basis for the text, the examples and the exercises presented in the book. While so many crystallography books are today rushed and published with a number of serious mistakes, both conceptual and typographic, here we have a counter-example where the long preparation resulted in a rigorous, carefully checked and polished text which, despite a few imperfections, looks like a time travel to another era when scientists were still able to devote enough time to think rather than running a black-box, to concentrate on scientific problems instead of administrative trivia, and to present their results when they were mature not when they had to be presented to meet a deadline. The reader should not be fooled: the travel back to another era concerns only the care by which the book was prepared; the content, far from being outdated, is of extreme actuality and should be taught in every advanced crystallography lecture. Unfortunately, in a world where it is difficult to defend teaching even of basic crystallography, advanced topics like this are systematically neglected. Now at least we have a reference text which, with its numerous examples and exercises, also perfectly fits the purpose of self-study, provided the reader is sufficiently familiar with space-group theory. This book is the perfect companion of Volume A1 of the *International Tables for Crystallography* and of the software routines available at the Bilbao Crystallographic Server.

After a short introduction (seven pages), with some historical remarks and a brief presentation of the fundamental ideas, the book is divided into two main parts, each subdivided into nine chapters: *Crystallographic Foundations* and *Symmetry Relations between Space Groups as a Tool to Disclose Connections between Crystal Structures*, followed by some historical remarks, four appendices, the last giving the solution to the exercises, a long list of references (399) and a glossary much welcome by the newcomer unfamiliar with the topics dealt with in this comprehensive text. The index is very detailed and spans six pages.

It is honestly difficult to find defects in this book, but because a book review would not deserve its title if it simply invited the reader to get a copy I had to find something to criticize; not an easy task. Actually, in a book published by IUCr one would expect that all the crystallographic standards are followed. Instead, lengths are given in pm rather than in Ångstroms: true, the latter is not officially in the international system, but it is the standard in crystallography, for obvious reasons.

The first part could ideally be extracted from the book and even separated in such a way that would be largely superior to most of the books that pretend to give an introduction to *Crystallographic Foundations*. Indeed, the title of this part is too humble; the topics presented go much farther than what is found in common crystallographic textbooks, up to the use of normalizers of space groups and the concept of conjugated subgroups and factor groups. These subjects should be part of the fundamental knowledge of any crystallographer, and in this respect the author is right in choosing the title: sadly enough, they are often considered 'esoteric' and almost systematically omitted in crystallography textbooks. For example, the topics of the equivalent description of crystal structures, of wrongly assigned space groups and of non-conventional settings of space groups are introduced in a synthetic but remarkably clear way. The presentation is rigorous yet it does not indulge in the sin of excessive formalism, which scares so many readers: it is proof that it is possible to be rigorous yet understandable and pedagogical.

Of special interest is the notion of *subgroups on a par*, possibly formally introduced here for the first time, although the concept is obviously not new. These are groups of the same type (same Hermann–Mauguin symbol), same cell parameters, which are not conjugate in the supergroup but in the Euclidean normaliser: they thus belong to different conjugacy classes. This type of subgroup occurs in the case of translational conjugation, *i.e.* when the ordering of atoms, which were statistically disordered in the supergroup, leads to a larger cell and to different choices of the origin, finally resulting in atomic distributions that are not related by the translations lost when going from the group to the subgroup. The importance of this concept when dealing with order–misorder phase transitions is self-evident. Note: The term 'misorder' is intro-

duced in this book to indicate a state of 'order with faults', which is opposite to complete disorder.

Because perfection does not belong in this world, even in this text a few imprecisions have to be pointed out: they are mainly concentrated in Chapter 6. At p. 68 we find some confusion between the notions of point group and crystal class. Point groups can be classified in point-group types, on the basis of which crystal classes are defined, but a crystal class is not a group. Therefore, the statement 'the crystal class is a (proper or improper) subgroup of the holohedry' is imprecise, the relation holding for groups but not for their classification in classes. In the same way, saying that there are classes that 'belong to point groups' is not correct because groups are classified in classes and not the other way round. Table 6.2 presents the metric restrictions on Bravais lattices in the same incorrect way as it appears in many textbooks. Indeed, while symmetry does impose equality of linear parameters or specific values of angular parameters, the lack of symmetry cannot impose inequalities or exclusion of special values. For example, it is incorrect to write that in a monoclinic lattice $\beta \neq 90^\circ$: the lack of symmetry restrictions allows β to take any value, including 90°. No distinction is made between 'crystal system' and 'lattice system', used interchangeably: a defect shared by many other textbooks.

A number of definitions and wordings are not fully satisfactory or incomplete. (1) Definition 2.6 is a non-definition of conventional bases: a true definition should have been given instead. (2) The definition of reciprocal lattice at p. 16 is far too synthetic: instead of referring the reader to a crystal-structure analysis book, a couple of pages could have been devoted to this topic. (3) Definition 2.9 introduces the 'lattices constants or (better)... lattice parameters'. Even better would have been to call them 'cell parameters' because the same lattice can be described by different cells having, obviously, different parameters. (4) Definition 3.1 of a crystallographic symmetry operation is a little too restrictive: it applies not only to crystal structures but also to crystal patterns. (5) When introducing the coordinates of a point with respect to the crystallographic basis, it would have been useful, for the beginners, to specify explicitly that these are fractional coordinates. (6) The term 'net plane' is used instead of the much more common 'lattice plane'. (7) The priority rules for space-group symbols are mentioned *en passant* at p. 71: it would have been better to give the sequence for mirror and glide planes as well. (8) A sentence explaining why $\bar{6}$ is used instead of 3/*m* would have been welcome (3 is compatible with both a hexagonal and rhombohedral lattice, whereas the horizontal *m* only with the former). (9) The term 'interchangeable' is used instead of 'commutative' at p. 56.

A curious mistake occurs in the caption of Fig. 4.1, which shows the effect of different symmetry operations on an asymmetric object. The example used is the Chinese character for 'point', for which the correct Chinese reading ('diǎn') is given whereas the Japanese reading is wrong (the correct reading is 'ten'; the word 'hoshee' used in the caption is a corruption of 'hoshi' which means star, not point, and corresponds to a completely different Chinese character).

The second part represents the reference for all those who need to understand and apply the symmetry relations between crystal structures. The author leads the reader on a step-by-step travel that requires a certain effort – examples have to be studied and digested, not just read - but is definitely rewarding. The reader will learn to derive the structure of a lower-symmetry phase obtained by a phase transition, to compute the atomic positions of a concrete structure from a structure type, to model the formation of transformation twins or antiphase domains, producing a structural model ready for the refinement against diffraction data. To follow the examples the reader needs to have to hand Vol. A1 of the *International Tables for Crystallography* (printed or online edition). He can also use the Bilbao Crystallographic Server, which is free of charge, but needs a bit of experience (number of schools are regularly organized which include practical sessions on use of the server). The examples proposed are based on the classical case of closest packing of spheres as an aristotype of non-molecular structures – from which the reader is going to learn much more than he may expect – and on the packing of molecular compounds. The only remark one may make on this section is that the presentation of structural data could have included the volume of the unit cell, to have a first idea of the type of structure–substructure relation to be studied.

Chapter 15 is an impressive summary of the theory of phase transitions, completed by additional considerations in *Appendix B*, where a wealth of concepts and definitions is presented in a clear and understandable way. The author emphasizes his well known position against the idea of the existence of a common subgroup in reconstructive phase transitions, while others affirm that this subgroup does not automatically mean the existence of a structural relation between the corresponding crystal structures (details on the different positions can be found in Chapter 1.7 of Vol. A1 of the *International Tables for Crystallography*).

Despite the clear, precise and rigorous presentation, a few terminological slips appear in the description of twins and antiphase domains: a confusion between twin law and twin operation, used interchangeably; the unfortunate term 'translation twins', used to indicate antiphase domains, contrary to the very precise and historically rooted definition of twins which nobody has the right to deform; the awkward expression 'merohedral twinning' used instead of 'twinning by merohedry' or 'merohedric twinning'. It is true that in German there is no distinction between these two adjectives, both corresponding to *meroedrisch*; however, a merohedral crystal can undergo twinning by merohedry or by reticular merohedry, leading either to an apparent pleonasm like a 'merohedral twin of a merohedral crystal' or to a semantic monster like a 'non-merohedral twin of a merohedral crystal'. The categorization of twins is also incomplete: mechanical twins as well as post-growth twins formed by oriented attachment are missing.

Chapter 18 goes deep in the algorithms of structure-type prediction *via* number theory: a nice complement which however requires some additional effort by the reader.

The care with which this book has been prepared clearly also appears in the almost complete absence of typos: the only one, really trivial, I could find is in the footnote at p. 24 ('by' instead of 'be').

In conclusion, this is a book that, despite a few terminological slips, every crystallographer taking seriously his job should have on his shelf.

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