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**Symmetry of Crystals and Molecules . By Mark Ladd.  
Oxford University Press, 2014. Pp. xxi + 433. Price  
GBP 55.00 (hardback). ISBN 978-0-19-967088-8.**

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► **To cite this version:**

Massimo Nespolo. Symmetry of Crystals and Molecules . By Mark Ladd. Oxford University Press, 2014. Pp. xxi + 433. Price GBP 55.00 (hardback). ISBN 978-0-19-967088-8.. Acta Crystallographica Section A: Foundations and Advances [2014-..], 2015, 71 (2), pp.250 - 252. 10.1107/S2053273315001916 . hal-01757634

**HAL Id: hal-01757634**

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Submitted on 3 Apr 2018

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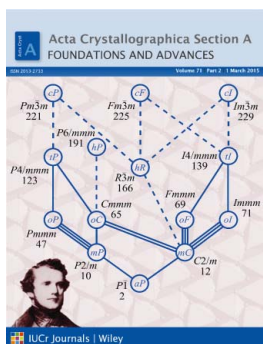
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*Acta Cryst.* (2015). A71, 250–252

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## Symmetry of Crystals and Molecules. By Mark Ladd. Oxford University Press, 2014. Pp. xxi + 433. Price GBP 55.00 (hardback). ISBN 978-0-19-967088-8.

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**Keywords:** book review; crystal symmetry; molecular symmetry.

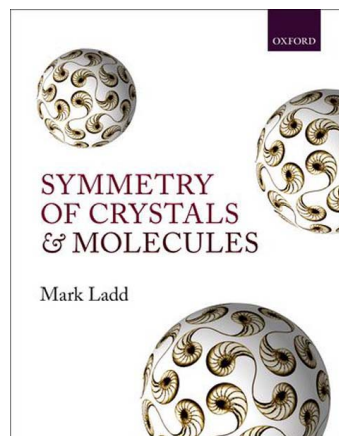
*Symmetry of Crystals and Molecules* is an ambitious textbook which tries to cover a wide range of topics, from the general idea of symmetry in Nature and art to the theory of irreducible representations. The presentation tries to be as pedagogical and illustrative as possible, without too much formalism. Unfortunately, the result too often lacks rigour and the (over)simplifications adopted to make the presentation light and accessible result in imprecision and the presence of real mistakes that noticeably reduce the value of the text. The systematic preference given to Schönflies notation over Hermann–Mauguin notation is impossible to understand or justify, and adds more confusion to a text that is already confused.

The book consists of nine chapters and 13 appendices, preceded by a list of ‘physical data, notation and online materials’, where an extensive list of symbols is presented in alphabetical order. The reader is quite often invited to use the online material referred to here.

The first chapter gives an overview of what symmetry is and of its ubiquitous presence in Nature and in the work of human ingenuity. From this very first chapter the reader is struck by a defect that affects the whole book: the use of undefined terms, such as body-centred and primitive unit cells mentioned here but defined only later.

The second chapter starts with a historical glimpse at the morphological basis of crystal symmetry and immediately introduces crystallographic axial settings, Miller and Miller–Bravais indices, the stereographic projection and, with a short jump in time, the reflecting goniometer. A few pages of calculations in stereographic projection follow, whose usefulness is doubtful: the use of the reciprocal lattice and the corresponding metric tensor would have made things much clearer, easier and more useful. But the metric tensor does not appear at all in this book. The noncrystallographic four-index notation for lattice directions, common in the metallurgical world, is used here: one of the many departures from the international standards. The rest of the chapter is devoted to molecular geometry on the basis of the valence-shell electron-pair repulsion theory. Some appreciable statistical treatment of experimental errors and their propagation is followed by seven pages about the Schrödinger equation and atomic and molecular orbitals, where a wealth of concepts are touched *en passant*, making this section obscure for a newcomer and useless for those familiar with the concepts. The chapter ends with three pages on crystal packing where the topic is just announced, rather than treated.

Chapter 3 deals with ‘point-group symmetry’ without having introduced the notion of a group (this will follow in Chapter 7), rather akin to building a house from the roof down. The restriction on rotational symmetry imposed by the periodicity is anticipated here, while lattices are introduced in the next chapter. Seven two-dimensional point groups out of ten are given in Table 3.1 (the full list is in Table 3.2), where the presence of a mirror in the second position for point group 4 and of mirrors in the second and third positions for point group 6 are clearly typographical errors. The (types of) crystallographic point groups are introduced *via* Euler construction: certainly not wrong, but to print a *new* text one should present something *new*, and there is certainly no shortage of more elegant and efficient ways of obtaining this result. Nonstandard graphics are used for the stereographic projection. The second part of the chapter deals with molecular point groups and physical properties, with brief definitions of enantiomorphism and chirality, two and a half pages about optical properties, and half a page about infrared and Raman activity (later presented in Chapter 8). A brief introduction to pyroelectricity and piezoelectricity



(just over a page) contains a fundamentally wrong statement about the piezoelectric effect: ‘The stress must be applied along a polar direction in the crystal.’ This is obviously not the case, otherwise crystals without a polar direction would be not able to show such an effect and there would be no symmetry difference between pyroelectricity and piezoelectricity. A few examples of molecules with their symmetry follow, then a section of 16 lines presents ‘noncrystallographic point groups’ for molecules (the user is invited to use the software). Hermann–Mauguin and Schönflies symbols are at last introduced (after having been extensively used in the previous 95 pages), followed by a section on the matrix representation of point-group symmetry operations *without* having introduced a suitable reference (the Bravais lattices). The chapter ends with nine pages about non-periodic crystals – and we are still waiting for lattices!

Chapter 4 finally introduces lattices, where a disturbing oscillation between lattice system and crystal system occurs here and there. The *hH* cell is introduced at p. 130 but not called this, a minor sin compared with the one that follows straight away, where we read about ‘trigonal lattices’, which of course do not exist: trigonal is a crystal system, in which the lattice can be hexagonal or rhombohedral. Bravais’ law, very briefly touched upon on p. 135, should have been explained in more depth and more clearly. The following four pages give a rushed introduction to the reciprocal lattice with the example of a monoclinic lattice: the general triclinic case would certainly have been too complex to introduce without the metric tensor. Next, we finally find the ‘rotational symmetry of lattices’ (read: restrictions imposed by periodicity), which should have come before point groups (the notion of group even earlier, of course). This is followed by ‘lattice transformations’, with basis vectors given as column matrices, at odds with crystallographic standards (in Eq. 7.8 the correct presentation is given instead).

Chapter 5 deals with ‘space groups’ (while we are still waiting for the definition of a group), including some discussion of reflection conditions, while diffraction is introduced only in the next chapter. An awkward statement appears here: ‘If a space group contains translational symmetry [...]’. One could bet a billion to one against finding a space group violating this condition and be sure to win. Axes are labelled as *x, y, z* instead of *a, b, c*, as used by ‘some authors’ (at least all those publishing in a crystallographic journal!). Several imprecise statements which would be too long to list occur across this chapter. An example of the derivation of symmetry operations from coordinate transformations follows: to place this material before the definition of a group (which follows in Chapter 7) is illogical. Then the reader suddenly meets the classical formula (Eq. 5.1) for calculating the crystal density: why here, in a section called ‘space groups related to point group  $2/m$ ’, is another mystery. A few lines are devoted to the concept of symmorphic space groups: contrary to many other books, which simply contain fundamental errors, here the definition is correct, although far from being the most general and useful one. On the contrary, the awkward term ‘point space groups’ to indicate symmorphic groups seems to be

newly coined here. Next, we find the ‘half-shift rule’, which aims to represent the fact that a symmetry element is repeated every half period. It is introduced in a section dealing with monoclinic space groups and thus it is not wrong. It is used also elsewhere, which may give the impression that is a general rule, while it applies only to twofold symmetry elements. For the orthorhombic groups some discussion of alternative settings is presented, which would have been much clearer with a bit of matrix algebra. A wrong interpretation of the reasons for the alternative choice of the origin in some space groups leads to wrong statements, like the assignment of two origin choices in space-group type  $I4_1$ , ‘either on  $4_1$  or on  $2$ ’ (p. 179); the only origin choice is actually on the twofold axis, because the site-symmetry group of a position on the fourfold screw axis is 1. Another awkward statement comes at p. 194, where we read that ‘space group  $P2_13$  [...], unlike  $P23$ , shows threefold axes other than those along  $\langle 111 \rangle$ ’. This is obviously wrong because threefold axes in cubic crystals are all along  $\langle 111 \rangle$  only (with respect to the conventional basis, of course). A really silly statement follows at p. 196, where we read that ‘cubic space groups of higher symmetry [...] are [...] not often encountered in practice’. NaCl (mentioned on the next page), diamond, PbS, metals, ...; the list of cubic holohedral compounds is far from being negligible! Section 5.5 finally gives a very short introduction to the matrix representation of symmetry operations: just two pages, which seems insufficient. This is followed by five and a half pages on di- and polychromatic symmetry, where imprecise language strikes again: ‘the fourfold rotation point at the centre of the unit cell is in a different orientation from those at the corners’. How a *point* could be characterized by an *orientation* is one of the several mysteries in this book. The chapter ends with a brief presentation (five pages) of *International Tables for Crystallography*, where the Seitz operator is used without being defined.

Chapter 6 deals with ‘symmetry and X-ray diffraction’. The Laue equations are not even mentioned, and Bragg’s law is derived without explaining why reflection can be used as an analogy for a diffraction phenomenon. The presence of the integer factor  $n$  in Bragg’s law is explained as coming from planes with interplanar distance  $d/n$  (which do not exist) instead of as the order of diffraction. If one pretends to reduce all the physics of the interaction between radiation and matter to two pages, these approximations are unavoidable, yet certainly not acceptable. The reciprocal space and Ewald’s sphere span just one page, then a few pages follow about experimental methods: Laue, precession, a few lines about the four-circle diffractometer which is essentially a matter of ‘sophisticated computer software’ – for the rest, the reader is sent to the literature. The structure factor pops up as a *deus ex machina* (no derivation), followed by the ‘limiting conditions’ (why change the name from systematic absences?) for a few examples derived analytically; use of a figure here would have made things clear. One page with the title ‘Using X-ray diffraction information’ suggests that the reader can determine the space-group type from the ‘limiting conditions’ on the basis of those few examples: hopeless!

Chapter 7 (44 pp.) covers 'elements of group theory'. After a brief introduction where *elements* and *operators* are incorrectly used as if they were synonyms and where a different classification of groups containing a  $\bar{6}$  axis in the Schönflies and Hermann–Mauguin notation (trigonal *versus* hexagonal) is pointed out but not explained, the group 'requirements' (read *axioms*) are introduced. The homomorphic condition should have been rigorously defined: it would have avoided a bad mistake (p. 245) when it is stated that 'every space group based on a given point group is isomorphous with that point group'. It goes without saying that an infinite (space) group cannot be isomorphic with a finite (point) group. Several pages are then devoted to the representation of point groups where the reader is struck again by a lack of rigour. For example, Eq. 7.15 and Eq. 7.17 are not *identical* but *equivalent* (the matrices indeed differ); the  $3 \times 3$  blocks in the structure of the  $9 \times 9$  matrices in Eq. 7.25 and Eq. 7.26 are *not* irreducible representations of  $C_{2v}$ , a statement contradicted four pages later (p. 261) where the character table of the group shows only four *one-dimensional* irreducible representations; the symbol  $A$  is attributed to the totally symmetric representation, which is an oversimplification because most groups contain more than one  $A$  representation. The presentation seems to oscillate between the temptation to present everything and the will to keep it light, so that eventually the reader is sent to 'more detailed analysis' in the literature. The expression 'Operations  $S_4$  and  $S_4^3$  do not combine in this point group' (p. 274) may give the wrong impression that they cannot act on the same set to produce another operation of the group, whereas what is meant here is that they are not conjugated.

Chapter 8 presents 'applications of group theory', where the section 'application to diffraction studies' gives a few examples of interatomic distances in simple compounds. This has no relation to the title, apart from a reference to another book by the same author (*et al.*). Next comes a section on 'application of theoretical studies', which is nothing more than a very brief (less than three pages) account of the MO–LCAO theory, and two brief accounts of Monte Carlo methods (17 lines) and molecular dynamics (35 lines), followed by a few examples of molecular-orbital analysis of small molecules ( $H_2O$ ,  $CH_4$ , benzene). Five pages introduce the basic ideas of crystal-field and ligand-field theories, with one example of  $[Fe(CN)_6]^{4-}$ . The next section is devoted to *vibrational studies*, where the classic example of the water molecule is presented first. The following example,  $BF_3$ , is problematic because it leads to the wrong decomposition of the reducible representations in  $2A_1' + 2E'$  instead of  $A_1' + A_2'' + 2E'$ : the problem is solved with a touch of a magic wand by saying the 'one result of  $A_1'$  is spurious'. A quick look at classical texts like Cotton's *Group Theory in Chemistry* gives the right result. The following three pages give a flavour of Raman spectroscopy and send the reader to the literature, before a short and intuitive (as

opposite to systematic) derivation of the crystallographic types of point group. The term *dihedral* is used for  $T$  and  $O$  cubic groups, which is far from being an acceptable approximation. Also, the use of roto-reflections makes the derivation somewhat problematic and leads to considering the point group  $S_4$  (*i.e.*  $\bar{4}$ ) as 'unique in that it cannot be determined by any other point group or combinations thereof': the use of  $\bar{4}$  instead of  $\sigma_h$  as generator would make things straightforward. The following section aims at giving an idea of the derivation of space groups, but again the lack of rigour and the departure from international standards is frustrating. The last two pages are a condensate of undefined terms and examples which give the strong impression that they have been put there because they needed to appear somewhere, but they are pretty useless for both the newcomer (who will not understand anything) and the experienced user (who will not get any insight into details nor find a smarter presentation).

The last chapter presents the set of computer programs available for download and is followed by the set of 13 appendices, before giving the solutions to the exercises. The index is quite complete, spanning 11 pp., although some entries are missing (for *Seitz operator* we find *see Symmetry, operator, Seitz*, but the latter does not exist).

A few typographical errors, like the trigonal and hexagonal systems counted as 'three [...] crystal systems' (p. 187), a closed curly bracket pairing an open round bracket (p. 188), 'produced' instead of 'produce' (p. 195), a missing comma (p. 251),  $C_2$  instead of  $D(C_2)$  (Eq. 7.12), a missing equals sign (Eq. 7.67), a missing word ('and two examples will be shortly' – what? p. 278),  $I_{21}3$  instead of  $I2_13$  (p. 324), are regrettable but do not represent a major obstacle to understanding. More serious are: the symbol for a zone axis  $[uvw]$  instead of that for a zone  $\{hkl\}$  (p. 30) and the opposite mistake at p. 88, where curly brackets (forms) are used instead of square brackets to indicate a direction; a square root is missing in Eq. 4.4; the typo  $C_{2v}$  instead of  $C_{2h}$  (p. 243); the  $\beta$  instead of  $\alpha$  in Eq. (7.64); the missing \* for complex conjugate in Eq. (7.47); the term irreducible instead of reducible (p. 271, just before Eq. 7.59); the incomplete Eq. (7.68), where ' $\mathbf{B} =$ ' after the symbol for the direct product is missing, giving the reader the impression that the  $\mathbf{A}$  matrix is multiplied by the result of the product; and the negative determinant used for the axial transformation (p. 326).

In summary, the scope of this book is clearly far too wide: the large number of topics cannot be presented in depth (the treatment of some just scratches the surface), and all suffer from approximations and lack of rigour. All that is presented here is already available, and in a much more precise and correct way, elsewhere, even if not necessarily in a single textbook. Once again, we face a modern book which by no means can stand next to many classical texts. The question then comes naturally to one's mind: who needs this book?