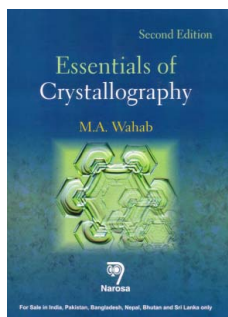# book reviews

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Essentials of Crystallography, second edition. By M. A. Wahab. Narosa Publishing House, 2014. Pp. xix + 335. Price USD 98.00 (North and South America), GBP 49.95 (rest of the World outside the Indian sub-continent). ISBN 978-1842658413 (outside the Indian sub-continent), 978-81-8487-316-0 (in the Indian sub-continent).

The review copy of *Essentials of Crystallography* I received from the publisher says 'for sale in India, Pakistan, Bangladesh, Nepal, Buthan and Sri Lanka only', appears as published in 2014 (I received it in summer 2013) and has an ISBN different from the international edition, which appears as published on 30 August 2013. The number of pages is the same and I assume that the content is also identical.

According to the preface and to the back cover, the second edition differs from the first one by the presence of a new chapter (No. 15) on representation of symmetry operations. We'll see that this chapter is a sort of 'dangling bond' rather disconnected from the rest of the book, whose presence is hard to justify.

The book consists of 15 chapters, which can be ideally divided into three parts: geometric crystallography (Chapters 1 to 7), crystal growth and defects (Chapters 8 to 9), diffraction and structure solution & refinement (Chapters 10 to 14), plus the new chapter on representations. From the very beginning – the preface to the second edition – the reader is struck by the unusually high number of typographical errors which, if they do not prevent the reader understanding the text (despite some really fantastic inventions like the 'refracture index'), show an unjustifiable lack of attention: the use of a spell-checker would have avoided the feeling of passing through a minefield. Adding to this the frequency with which the reader will leap from their seat when reading incorrect, badly worded or outdated statements, it is advisable to wear robust protection before approaching this book. Also, many references quoted in the text do not appear in the bibliography, which is very short and quotes old and outdated editions (the first edition of Giacovazzo's book; the 1965 'red' edition of *International Tables*).

The geometric crystallographic part contains classical material available in countless texts, many of which are more rigorous, precise and detailed. No use of the metric tensor is made, and this leads to several lengthy and unnecessary trigonometric calculations. A defect this book shares with (too) many others is the confusion between the concepts of crystal system and symmetry of the lattice. For example, the terms 'trigonal' and 'rhombohedral' are used as if they were synonyms; the inequalities of parameters of a lattice are transferred as such to the crystal systems, ruling out implicitly the cases of metric specialization, which are far from rare.

Quite disturbing is the confusion between atomic position and lattice node. The expression 'a crystal structure is formed only when an atom or a group of atoms (or molecules) is attached to each and every lattice points' (p. 3) gives the reader the wrong impression that the two concepts coincide, but it could just be an unfortunate choice of wording. However, the definition of 'linear and planar atomic density' (p. 12), where the lattice parameters are used to compute the number of atoms along a direction in a plane without any reference to the Wyckoff positions (the lattice nodes are obviously meant here) emphasizes this confusion, and the awkward expression 'coordination number of a given lattice' (p. 13) makes the fog even denser. Again, atoms and (lattice) points are treated as synonyms in the discussion of centred three-dimensional cells, and the packing efficiency of simple, body-centred and face-centred *structures* are discussed in a chapter on *lattices*.

The cubic system is termed 'the most symmetric of all crystal systems' (again in Chapter 5), which is not correct because cubic groups are not supergroups of hexagonal groups. The fact that the holohedry of highest order occurs in the cubic system is obviously meant here, but the expression is unfortunate and incorrect.

Chapter 3 deals with symmetry *elements* in two dimensions and contains a number of mistakes. No distinction is made between symmetry *elements* and symmetry *operations*; this leads to the aberration of using the term 'element' even for the translations, which are operations that do not have symmetry elements. Translations are incorrectly included among the symmetry operations of 'a two-dimensional object (or a regular body)', which is of course wrong because only an infinite pattern can be compatible with a translation. This error occurs again (p. 44) when translations show up again in the list of *macroscopic* symmetry elements (strangely enough, they are not present when discussing the three-dimensional macroscopic symmetry, in Chapter 4). Rotation *axes* are used in a two-dimensional space where the lack of the third dimension makes them simply rotation *points*. The notion of group is used without being defined but referring the reader to the 'mathematical sense'.

The reader will (hopefully!) leap from their seat when reading the following sentence (p. 47): 'A combination of proper rotations with translations yields complex symmetry groups which leave space unmoved and these are accordingly called space groups.' Where an inherent oxymoron like a translation leaving any point in space unmoved (let alone the

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whole space) could have come from is one of the many mysteries in this book. Perhaps it comes from a semantic joke: if a *point* group leaves a point unmoved, then a *space* group must leave the space unmoved; brilliant! Another exploit is the introduction of a *triangular* unit cell in the two-dimensional space (p. 54); how a geometric form with only three corners could represent a translational unit is another mystery engraved in this chapter.

Chapter 4 deals with symmetry in three dimensions. The rotoinversions are missing from the list on p. 60 and again at p. 62, although they appear in Fig. 4.2. The rotations are defined as 'about a point', while they are about an axis (the opposite error occurs in the previous chapter, as we have seen). Point groups are introduced with a presentation, rather than a demonstration, *via* Euler's construction passing through 'monoaxial combinations' and 'polyaxial combinations', which lead to symbols like 322, 332, 233, $\bar{n}2\bar{2}$ and so on, which certainly create confusion in the newcomer: a more modern and standard presentation would have been preferable. Rotoreflections (not used in crystallography) are introduced before rotoinversions. The left and right parts of Fig. 4.10 are expected to give 'alternative demonstrations', but actually the right part is the same as the left part, just with the mirror removed. The terms 'crystal class' and 'point group' are incorrectly treated as synonymous.

Chapter 5 is a lengthy derivation of the crystallographic point-group types, which would raise many eyebrows if we had more than two. Terms like *holohedric* (misspelled for *holohedral*, later *holosymmetry*, a remnant of old texts) and *Laue group* are used before being defined. Groups containing vertical mirror and rotoinversion axes (called *XXXm* groups) are derived from holoaxial groups (222, 32 and 23) by placing a mirror 'parallel to the combination' of axes. If one has to understand the 'combination' as 'intersection' of the axes, then this sentence does not make any sense, the intersection being a point. Actually, these mirrors have to be added, so that each of them contains the axis of higher order and is perpendicular to one of the other axes, but this is not at all evident from the sentence above. Furthermore, the non-existing group $\bar{3}2m$ (not a typographical error for $\bar{3}2/m$, given right after that as $\bar{3}m$) shows up in the list. The classical confusion between crystal system, lattice system and Bravais lattice occurs in Table 5.11, where the unnecessary metric restrictions are given for the definition of a crystal system (the presence of a symmetry operation results in specific value of the lattice parameters, but the *absence* of symmetry operations does not preclude particular values or relations among lattice parameters) and the terms 'trigonal' and 'rhombohedral' are again wrongly treated as synonyms. Section 5.4 introduces 'linear orthogonal transformations', with a huge slip. The coordinate transformation due to a change of basis is given as $x'_i = \sum_{j=1}^{3} C_{ij}x_j$, with $C_{ij} = 1$ for $i = j$ and 0 for $i \neq j$; in other words, the transformation matrix is the identity matrix, *i.e.* no transformation at all! Table 5.7 is the multiplication table of point group 4, not the character table, as incorrectly stated in the caption as well as in the text mentioning the table. The derivation of point groups is performed by obtaining the

intermediate symmetries between the 'essential symmetry' (undefined: it must be the minimal set of symmetry elements common to a crystal symmetry) and the 'holosymmetry' (read *holohedry*). The crystal system is now defined in terms of the shape of the unit cell: it is thus a crystal family (if it is the conventional unit cell) or a lattice system (if it is the primitive unit cell). The reader will (should!) leap from their seat on reading that 23 is a short notation for 233 and that 432 is shortened to 32 (*sic*!). The chapter ends with a brief introducion to the Laue symmetry, where we read about anomalous *diffraction*, and to the concept of crystal class, wrongly used as a synonym of point group (a crystal class *classifies* point groups in types). Finally, in the appendices we find the direction [000] for triclinic crystals, instead of the statement that no symmetry direction is defined in this case.

Chapter 6 is devoted to the derivation of space groups and consists of 13 pages, just a little over a third of the number of pages devoted to point groups (35 pp.). Obviously, space groups are not 'derived' but just briefly presented. After giving the number of types of screw axes and glide planes (for the latter, a wrong number, five instead of six, is given; the *e* glide is still absent in a text published in 2014!), these are briefly presented and summarized in two tables (6.1 and 6.2), where almost half of the graphic symbols are missing, replaced by a segment. The reader discovers here the existence of general and special position as an exclusive feature of space groups (p. 117), while these obviously also occur in point groups. Special positions are then defined as being on symmetry elements, without making any distinction between those with and without a translational component. This component immediately reappears, however, in the cryptic sentence 'The space groups either lack a translation component or in some cases despite having a translation component, certain pairs (or sets) of points are found to coalesce.' How a space group, which by definition is built on an infinite set of translations, could 'lack a translation component' will remain forever a mystery. This is followed by a section on systematic absences (why here, before introducing the reciprocal lattice and diffraction, is just one of the many incoherencies of this text) through a series of statements, without any demonstration (not even 'presentation'), where reflections are given between parentheses as if they were families of lattice planes. Zonal and serial conditions (never called this) are said to occur 'when a crystal [. . .] is held in certain orientation', which gives the reader the impression of complete subjectivity. Here what is meant is obviously the fact that these reflection conditions come from the projections of symmetry operations with a translation component, but those who do not already understand the reflections conditions will never guess this from the presentation, while those who know them leap once more from their seats. There is no time to sit down again, as another leap waits for the reader when they discover that '(*h*00) planes are perpendicular to *x*', which is perfectly wrong in three of the six crystal families. The definition of symmorphic and non-symmorphic space groups, which is often a trap for many books, is again wrong. Here the former is saved for a corner ('may be entirely specified by symmetry operations all acting

at a common point only' is not incorrect if those operations are the generators), but the goalkeeper could do nothing about the non-symmorphic groups, defined as space groups which 'involve the existence of microscopic symmetry elements such as screw axes and glide planes', a feature far from being characteristic of non-symmorphic groups only (a quick look at the diagram of *Cmmm* or *P4mm*, for example, would remove any doubt). The equivalence of unit cells for tetragonal lattices is wrong: *C* is not equivalent to *I* and *F* but to *P*.

Chapter 7 has the title *Crystal planes, directions and projections*, but a more precise title would have been *Crystallographic calculations*, which are made more complex than necessary by the absence of the metric tensor. As a consequence, only high-symmetry examples (cubic, hexagonal, rhombohedral) are given. The standard convention of writing covariant components as row matrices is not followed: instead, only column matrices are used. A very brief introduction to crystal projections is given and is definitely insufficient: nine lines and one equation for the stereographic projection, the same for the gnomonic projection, a little more for the spherical projection. The chapter ends with six pages where the reciprocal lattice is introduced without following the crystallographic standards (the dot product of vectors in the dual spaces is given as 2π instead of 1) and applied to a few simple cases (again, the metric tensor would have made things simpler and more general).

Chapter 8 presents methods of crystal growth, followed by thermodynamic considerations about nucleation and growth, which naturally dilutes the following chapter dealing with crystal imperfections. The discussion is centred on high-symmetry crystals of simple compounds (metals, halides), from which the reader may get the wrong idea that twinning and stacking faults are observed only or almost exclusively in close-packed structures (p. 205), which is of course wrong.

In the rest of the book, diffraction theory and methods are approached. Chapter 10 deals with the basics of diffraction geometry and presents powder diffraction and some old single-crystal methods (Laue, rotation/oscillation, Weissenberg, precession, very briefly); for details, the reader is referred to 'standard texts'. Diffractometers (powder and single-crystal, with point detectors only) are presented in just two pages (*versus* 25 pp. for film methods). Neutron and electron diffraction are presented in two pages, synchrotron radiation is mentioned once.

Chapter 11 deals with factors affecting the intensities and data reduction. The structure factor is introduced as a *deus ex machina*, without any explanation or derivation. The chapter ends with the agreement factor *R*, which has nothing to do here; it should appear later, when dealing with structure refinement.

Chapter 12 deals with 'structure factors and Fourier synthesis'. The reason for putting this chapter *after* the previous one, where the structure factors are used but undefined, is obscure to say the least. The reflection conditions are called 'special structure factors' and are derived only analytically for simple cases. The effect of a centred cell on the reflection conditions is presented only for *I* and *F* centring as if

it were a feature of cubic crystals, whereas it does not depend at all on symmetry. The word 'extinction' is incorrectly used for 'absence'.

The title of Chapter 13 is *Crystal structure analysis*, but actually it deals with structure *solution*. Trial and error is mentioned, and a few pages are devoted to Patterson and direct methods, but there is nothing about charge flipping. The following chapter ends this part with basic ideas about least-squares structure refinement and the use of Fourier difference maps to identify missing or displaced atoms and atoms needing anisotropic description of their thermal displacement. No figures of merits are discussed and, as seen above, the agreement factor *R* is introduced in Chapter 11, for unknown reasons.

Chapter 15 presents the basic ideas of representation theory of point groups. Although the introduction makes the reader eager for applications to 'physical and chemical problems', nothing is given beyond the construction of the character tables. A serious mistake occurs at p. 312, where it is stated that 'point groups and space groups are finite groups': a group containing an *infinite* set of translations could be *finite* only in the mind of Tertullian, who could here apply his well known statement *prorsus credibile est, quia ineptum est*.

The frequent use of nonstandard terms and conventions throughout the book, as well as the use of undefined terms, or of terms which are defined after being used, is quite annoying. The term 'lattice array' is used instead of 'crystal pattern'. The term 'natural axial systems' is used but not defined. The acronyms *bcc* and *fcc* are used before being defined (in the caption of Fig. 2.5). The interplanar spacing is introduced briefly in Chapter 2 in terms of the reciprocal lattice, which is instead introduced only in Chapter 7. International standards are not respected. For example, the axes are labelled as *x, y, z* instead of *a, b, c*. The *c*-unique setting of monoclinic crystals is constantly adopted. White symbols are used for rotation axes instead of standard black symbols (p. 47). Two-digit symbols are used for orthorhombic, tetragonal and hexagonal groups when the third one is not a generator: a remnant of the old standard abandoned long ago. The italic font style for letters in the Hermann–Maugin symbols is missing in Table 3.7. The orientation of twofold axis symbols change with their position in the unit cell. Plane groups *p*1 and *p*2 are written p_1 and p_2 (p. 56). Symbols for centrosymmetric cubic point groups are given with 3 instead of $\bar{3}$, as in the old (red) *International Tables*. The term 'Miller indices' is incorrectly used for the indices of direction as well. The *A*-centred space groups, which do occur as a standard setting in the orthorhombic system, are ignored, *P, C, I* and *F* being given as the only choice of unit cells in *International Tables*, which is of course wrong.

Overall, this book does not add anything but noise to the already crowded panorama of basic crystallographic textbooks. For example, Buerger's classical textbooks do a much better job, despite their venerable age. A book published in 2014 should be more up-to-date and modern, whether in the theory or in the description of experimental techniques (or both, of course), and cannot contain mistakes that one does not find in books half a century older, or more. The impressive

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number of typographical errors and the departure from IUCr standards make the reader think that the text has been rushed, despite being already at its second edition.

There exist several texts which, even if not perfect, remain a reference for students and scholars. These could be surpassed by a modern rigorous formulation covering new or rarely presented topics. *Essentials of Crystallography* is as far as one could imagine from this target. There was no reason to publish such a text. There is certainly no reason to buy it.

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