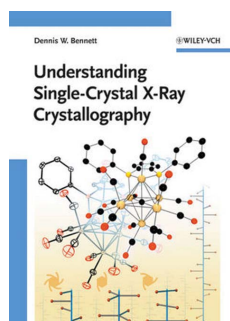


book reviews

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**Understanding Single-Crystal X-ray**

Crystallography. By Dennis W. Bennett. Weinheim: Wiley-VCH, 2010. Pp. xx + 811. Price (hardcover) GBP 115.00, EUR 138.00. ISBN 978-3-527-32677-8.

This 800-page book has been written for graduate students in biology or chemistry who lack any background in basic physics and mathematics. This ambitious aim is therefore to bring students from total ignorance of crys-

tallography, physics and mathematics to a good practical knowledge and understanding of crystallographic methods.

As the level of the reader is assumed to be low, all the mathematics, physics and statistics needed are developed in the core of the book, not, as is more usual, in appendices; therefore it is rather boring for readers who are familiar with some mathematics and physics (for example, dot and vector products in orthogonal space, basic linear algebra, Coulomb's law, wave definitions and so on) and the mathematical demonstrations are very lengthy. Furthermore, the use of trigonometry functions instead of complex exponentials does not help a beginner.

This overly long book is composed of eight chapters. The first two chapters (200 pp.) introduce geometrical crystallography, lattices and group theory. Most of the section on vectors in crystallography (20 pp.) describes the dot product and vector product using Cartesian coordinates, although the difficulty for beginners is usually in dealing with non-orthogonal lattices. The metric tensor and its use are not introduced. Elementary algebra applications are, for example, rotation matrices for threefold rotation in orthogonal space where the coefficients are not integer, but not in hexagonal or cubic lattices where the matrix coefficients are integer due to the properties of the lattices (this would have been an excellent way to introduce crystallographic rotation matrices). Section 1.5 describes coordinate systems in crystallography, but the metric tensor is not used, and for all calculations, including bond-length calculations, it is proposed that a transformation from the non-orthonormal crystal system to Cartesian coordinates is made before calculating the scalar product, instead of performing directly a dot product in crystal space. The same type of calculation is proposed for cell transformations. I recommend that the author reads the excellent book *Vectors and Tensors in Crystallography* by D. E. Sands and *International Tables for Crystallography* before writing a second edition.

Chapter 2 describes crystal symmetry and group theory using mostly Schoenflies notation, whereas crystallographers

use Hermann–Mauguin notation. Matrix notation is only given for orthonormal spaces, and there is some confusion between lattices and basis sets. The crystal classes are not defined. The representations of the point groups as stereographic projections do not follow the conventions of *International Tables for Crystallography* for the rotation axis, the stereograms and associated tables often contain errors, the author does not make a clear distinction between operator and operation, it is stated that there are eight threefold axes in cubic point groups instead of four, the total number of operations seems to be 45 instead of 48 in the point group $m\bar{3}m$ (not $m3m$), some diagonal mirrors do not exist, and so on.

The section on space groups is better and smoothly introduces all the concepts necessary to ensure that the reader is ready to understand Volume A of *International Tables for Crystallography*. But this is intended for chemists and biologists, who are interested in molecular crystals, not material scientists. Subgroup relationships are not mentioned. Once again, using the Cartesian coordinates to transform the rhombohedral lattice to a hexagonal one is not the easiest way.

Chapters 3 to 8 are devoted to X-ray crystallography for crystal structure solution and refinement. The theory is extremely difficult to follow, starting from Coulomb's law (not named as such) to charge-density calculation with a very lengthy and not always physically correct introduction to wave theory. Never in this chapter is it shown that the diffracted amplitude (which is written with an arrow?) is proportional to the product of two complex quantities: the interference function, which leads to the diffraction conditions for a perfect lattice, and the structure factor, which is the scattering term also used in gas, liquid and amorphous scattering theories. Furthermore, too many mathematical derivations use trigonometric functions instead of complex exponentials. I believe that X-ray diffraction theory should be taught starting from Thomson scattering, then defining interference between waves scattered by two electrons, then introducing the atomic scattering factor and the structure factor (with an application to gas scattering), and ending with the interference function in one-, two- and three-dimensional space. This approach would be much better than mixing all these concepts in two chapters (Chapters 3 and 4). Using my preferred approach, Laue's diffraction conditions, the reciprocal lattice, Bragg's law and the Ewald sphere emerge naturally.

Chapter 4 describes experimental methods, including old ones like the Weissenberg or precession methods, but not mentioning synchrotron radiation. The paragraph describing the four-circle diffractometer is correct but too long for beginners. As mentioned above, this chapter finishes with Thomson scattering (although not named as such), the inter-

ference function and anomalous scattering, which should have been introduced earlier in the book.

The first 40 pages of Chapter 5 are devoted to basic statistics before describing absorption, extinction, intensity scaling, anomalous dispersion, systematic absences and anisotropic displacement parameters, although not always in a sensible order (extinction and anisotropic displacement parameters are estimated and modelled *a posteriori*). Chapter 6 is a very long chapter devoted to experimental crystal structure solution and covers the Patterson function and its applications. Direct methods are described in great detail in Chapter 7, which is perhaps not necessary for beginners who do not know basic mathematics.

Chapter 8 discusses least-squares refinement and is quite long; however, this subject must be explained clearly to those who wish to practise crystallography and here it is done well: linear least squares and its applications, and nonlinear least squares applied to structure refinement (theory, weighting schemes, constraints, restraints, rigid groups, hydrogen atoms, twins and chirality) are all covered. I recommend this chapter.

In conclusion, this book could be useful to staff crystallographers who want to know more about direct methods or least squares and who have enough knowledge of crystallography to find the good chapters. But I do not recommend this lengthy and sometimes approximate book to PhD students or researchers in chemistry or biology who would like to understand how to solve a crystal structure: the logic and the physics of the part describing X-ray diffraction is very troublesome with too much detail, and the part describing geometrical crystallography is not clear and sometimes wrong. This is a real pity, because the crystallography community needs an excellent up-to-date book. In my opinion, though, it is not this book.

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