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Book and Media Review

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# Review of *X-Ray Crystallography*

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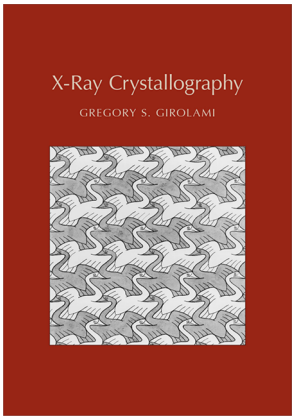
**X-Ray Crystallography**, by Gregory S. Girolami. University Science Books: Mill Valley, California, 2015. 300 pp. ISBN 9781891389771 (hardcover). $88.

Gregory Girolami's *X-Ray Crystallography* is intended to accompany an introductory, graduate-level course in single-crystal diffraction methods. His book is separated into three sections: Symmetry and Space Groups, Chapters 2−12; X-rays and Diffraction, Chapters 13−27; and Solving and Refining Crystal Structures, Chapters 28−40. Chapter 1 provides a brief history of crystallography. Chapter 41 describes powder diffraction; Chapter 42 describes electron and neutron diffraction. In general, the information is presented in a clear and sometimes unique manner. His many worked examples throughout the book and problems included at the end of each chapter help clarify descriptions of the theory.

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Some of Girolami's most unique presentations are in the chapters discussing symmetry. His initial definitions of symmetry terms in Chapter 2 are very rigorous. Luckily, the text following each of the definitions presents the concepts of the definitions in easy-to-understand forms. He uses a novel term, "traveling symmetry", to describe symmetry operations that combine rotation with translation, which is described in Chapter 5.

In a curious twist, Girolami uses orthographic projections in Chapters 2 and 3 to illustrate unique positions of point groups, as opposed to the more typical stereographic projections. However, it appears that the orthographic projections that he does include are identical to stereographic projections. None of the projections of the five cubic point groups are presented in this book. Also, he does not tell the reader how his projections are created, and he does not illustrate the locations of symmetry elements in any projections.

The remainder of the symmetry section, Chapters 8−12, describes the 2-dimensional plane groups and 3-dimensional space groups. Techniques to identify symmetry operations in the diffraction data and, hence, methods to determine space groups, are left until Chapters 26 and 27 after a discussion of the diffraction process.

The section on X-rays and diffraction starts with describing how to generate X-rays, Chapter 13, and how to measure and reduce diffraction data, Chapters 14 and 15. His description of the physics of X-ray generation is clear and complete. The book describes most of the instruments in use today, but does not include any description of liquid-anode X-ray sources, and only briefly mentions the new "photon counter" detectors. The equations used in data reduction that he presents are actually intended for point detector instruments. Similar but much more complicated formulas can be derived for modern area-detector instruments.

Girolami begins his discussion of diffraction by describing Thomson scattering from a free electron, Chapter 16, and then Rayleigh and resonant scattering from an individual atom, Chapter 17. His description of diffraction from a single row of scatterers, Chapter 18, is difficult to understand because there is no real-world example of this type of diffraction. Chapter 19 on diffraction from 2- and 3-dimensional arrays is more easily understood by having clear, real-world examples.

Chapter 22 on the limiting sphere and resolution includes definitions that may confuse students. According to the author, "measurable reflections" are "reflections that are strong enough that the intensity is measurably nonzero (i.e., larger than the noise of the detector)." Most crystallographers use the term "measurable reflections" to describe the data that can be measured with the current instrument set up, and use the term "observed reflections" to describe the spots that have some intensity value that is above the local background intensity.

His description of structure factors and phase angles, Chapter 23, is complete and mathematically rigorous. The drawings of layers of diffraction data for different Laue classes in Chapter 24 clearly demonstrates the various symmetries of the reciprocal lattices. The Flack parameter, described in Chapter 25, is the most accepted method of correctly determining the absolute structure of a material. However, no mention is made of the Hooft method, currently the most sensitive analysis for determining the absolute structure of a sample with weak anomalous scattering.

The structure solution methods discussed include trial and error such as molecular replacement (Chapter 29), charge flipping (Chapter 30), Patterson (Chapters 31 and 32), isomorphous replacement and anomalous dispersion methods for macromolecular samples (Chapter 33), and direct methods (Chapters 34 and 35). The next chapter describes modeling electron density, including disorder. Chapter 37 on refinement





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primarily covers least-squares refinement, but does briefly describe simulated annealing and maximum likelihood methods used mostly for refining macromolecular materials. Twinning of all types are covered, with several valuable examples in Chapters 38 and 39. A very useful chapter on mistakes and pitfalls follows in Chapter 40.

Chapter 41 on powder diffraction and Chapter 42 on electron and neutron diffraction explain the basic experiments of these areas as well as the general benefits and weaknesses of these types of studies. The book is concluded with appendices on vector manipulations, complex number mathematics, the Ewald sphere, atomic form factors, the Patterson function, an in-class demonstration of diffraction, and a brief bibliography.

*X-Ray Crystallography* uses a mathematical approach to symmetry and the fundamentals of X-ray diffraction. Although the author provides a number of real-world examples in the text and in problems for the reader, he focuses more on theory rather than on practice. This book could be a valuable text for a lecture course in crystallography.

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### Notes

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