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Book Review

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Crystal Structure Analysis. Principles and Practice, second edition, A. J. Blake, W. Clegg, J. M. Cole, J. S. O. Evans, P. Main, S. Parsons, & D. J. Watkin, Oxford University Press, 2009; ISBN: 9780199219476; 352 pp.; $59.95.

The field of structure solution and examination using X-ray diffraction has undergone significant advances during the last decade. The emergence of charge coupled device (CCD) area detector technology and less expensive and more powerful computer processing units have meant, on the one hand, that X-ray data and instrumentation are more accessible, whereas, on the other hand, the customary approach of carefully examining and weighing individual pieces of data pertaining to an X-ray data collection can fall pray to automation. The second edition of *Crystal Structure Analysis. Principles and Practice* is a book—as well as a guide—that does a remarkable job covering the fundamentals of the field while bringing the reader up to date on latest developments in a variety of subareas.

The book consists of 22 chapters and two appendices. As discussed in the preface, the book was originally derived from a course in X-ray structure analysis organized on behalf of the Chemical Crystallography Group of the British Crystallographic Association and held every 2 years from 1987. As such, there are contributions from a total of seven authorities—Alexander Blake, William Clegg, Jacqueline Cole, John Evans, Peter Main, Simon Parsons, and David Watkin—that address topics ranging from fundamentals and basics of diffraction to crystal growth and from data processing and refinement to structure analyses.

Having originated from a course, the general purpose of the book is to provide students with comprehensive coverage of all aspects of X-ray diffraction. The book greatly succeeds at this didactic endeavor. Chapters 1 and 2 provide an introduction to fundamentals of X-ray diffraction that is designed to bring the reader up to speed on the most important concepts. The authors recognize that is not necessarily important to digest all information at once, while making reference to the fact that much is learned during the process of collecting and analyzing data in the laboratory. References to other relevant sections within the book are also given at the beginning and in subsequent chapters. Chapter 3 then moves to the synthetic laboratory to discuss crystal growth. Various methods to grow crystals (*e.g.*, solvent evaporation, sublimation) are covered with an important transition to crystal mounting for data collection.

Chapters 4 to 6 address aspects of space-group determination (Chapter 4) and data collection (Chapters 5 and 6). In addition to discussing fundamental topics such as Laue symmetry and systematic absences, the chapter that covers space-group determination provides an introduction to *International Tables for Crystallography. Volume A*—a principal text for any diffraction laboratory. The chapters on data collection cover both fundamental and practical aspects that include a discussion

on the relation between real space and reciprocal space and problems encountered during crystal screening (*e.g.*, indexing).

Chapters 7 to 13 discuss data processing (Chapter 7), structure solution (Chapters 8 to 10), and structure refinement (Chapters 11 to 13). Throughout these chapters, the authors draw on experience related to areas such as twinning, structure solutions using Patterson maps, and electron-density map interpretation using examples from the laboratory. Fundamental mathematical relationships that define these areas are discussed with the recognition that care must be taken when relying on computer software to perform underlying calculations. As with the previous chapters, approximately three to four instructive exercises are given at the end of each chapter to encourage student participation. The chapter on structure refinement provides a very useful message that one must also take great care in deciding when refinement is complete, particularly in the context of assessing the quality of the X-ray data and the degree to which the structure makes "chemical sense."

Chapters 14 to 16 cover the interpretation of the results. A more specialized treatment on interpreting extended inorganic structures (Chapter 14) is provided, which is timely given recent interest in the related areas of coordination polymers and metal-organic framework materials. The purpose of the chapter is to also convey that what may seem as a crystallographic nuance (*e.g.*, site occupancies) can have a profound impact on the interpretation of the properties solids (*e.g.*, magnetic). Discussions are provided on analyzing results as related to molecular confirmation, hydrogen bonding, and thermal displacement parameters (Chapter 15). A very useful chapter on the meaning and significance of random and systematic errors is also given as related to the quality of X-ray data (Chapter 16).

Chapters 17 and 18 address power X-ray diffraction and twinning, respectively. As discussed by the authors, both areas have experienced increased attention in recent years. Indeed, it is now possible to solve very complicated organic structures using powder diffraction, and area detectors are now facilitating the detection of cases of twinning that may have previously gone unnoticed. Importantly, the authors discuss how computer software has evolved to meet demands of each area. Numerous examples of twin law derivations from the laboratory are given.

Chapters 19 to 21 cover aspects of presenting results (Chapter 19), understanding the crystallographic information (CIF) file (Chapter 20), and crystallographic databases (Chapter 21). Advice on selecting the most appropriate model for a presentation is given, as well as hints on presentations in journals and theses, as well as poster and oral presentations. The basics of CIF files are outlined and a clear treatment on the importance of depositing data to various crystallographic databases is provided. Chapter 22 then concludes with an overview on X-ray and neutron sources with a perspective on the global development of synchrotron X-ray sources and the utility of neutron diffraction. The two appendices supplement the text by providing primers on mathematics (*e.g.*, vectors, complex numbers) and various formulae.

The strength of *Crystal Structure Analysis. Principles and Practice, second edition*, lies in a careful consideration to balance theory and practice while being, at the same time, comprehensive. Indeed, the field of crystal structure determination requires input from participants with a diverse background. In a simplest scenario, a chemist with synthetic expertise makes a new compound and grows crystals while a crystallographer selects and mounts a crystal, as well as collects and solve the data. Both, of course will participate in the interpretation and dissemination of the data. In the ideal case, both are required to work in harmony in order to arrive at the most

accurate and meaningful conculsions in the context of a tested hypothesis. In this regard, *Crystal Structure Analysis* succeeds in uniting both perspectives so that the field of X-ray structure analysis can be expected to be ably cultivated for years to come.

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