

See ACA Newsletter, SPRING 2008

The 10 “must” read book list for X-ray Crystallographers.

As I was sitting in my office, at Texas A & M University, pondering where I was going to go for lunch, a student approached and we began a conversation on X-ray crystallography. The student asked a very interesting question, he said, "Given my limited lifespan (only 70 or so more years), I can only afford to read ten books on any given subject. What ten books on X-ray crystallography would you recommend?" Unfortunately the answer that I gave the student was unsatisfactory, due to the fact I was overwhelmed by hunger and I vowed to find a better answer.

With this in mind, I posted the same question to my colleagues on a user group newserver. The response that I saw was fantastic and here is the list that we produced. Keep in mind that this is an informal survey of very wise old masters with many years of research and teaching under their ever-expanding belts and as such there may be a few good books that we have not included. I call this the "must read book list" and I recommend that students and experts alike should consider this list when choosing their top ten books to read on the subject of X-ray crystallography.

The books are listed in no particular order. The remarks are from actual readers and do not necessarily reflect my opinion, but who am I to disagree with the old masters.

1. Crystal Structure Determination by: Werner Massa (March 31, 2004)
ISBN-10: 3540206442
“My favorite introduction to Crystallography.”
“It's the one book I would force into a student hands!”
2. Crystal Structure Analysis by: Jenny Glusker and Kenneth Trueblood (August 1992)
ISBN-10: 0195035313
“A good starter for the common scientist.”
3. Crystal Structure Analysis: Principles and Practice (International Union of Crystallography Monographs on Crystallography) by Peter Main, William Clegg, Alexander J. Blake, Robert O. Gould. (January 28, 2002)
ISBN-10: 019850618X
“One of my favorite and informative book(s).”
“Crystallographers should read this book first.”
4. The Determination of Crystals Structures by: H. Lipson & W. Cochran (June 1966)
ISBN-10: 080140276X
“It is still an amazing book!”
“Today's crystallographers could garner a new perspective and appreciation of the subject.”
5. Fundamentals of Powder Diffraction and Structural Characterization of Materials by: Vitalij Pecharsky and Peter Zavalij (March 3, 2005)

- ISBN-10: 0387241477
“Only book that I know of that explains indexing and indexing programs.”
“A must own book for the powder and single-crystal diffractionist!”
“A gotta-have book for people interested in the bigger picture.”
6. Structure Determination by X-ray Crystallography by: Mark Ladd and Rex Palmer
(September 30, 2003)
ISBN-10: 0306474549
“I have given Ladd and Palmer to non-crystallographers who needed to gain a basic understanding of the process.”
7. X-ray Structure Determination by: George Stout and Lyle Jensen (April 24, 1989)
ISBN-10: 0471607118
“A good, practical book for the student after they are into the subject.”
“My first book and the most recent book I have re-read on crystallography!”
8. X-ray Analysis and the Structure of Organic Molecules by: Jack Dunitz (December 16, 1996)
ISBN-10: 3906390144
“A great book (even for an inorganic chemist) and it is filled Jack's usual wit!”
“The section on weighting schemes in least squares is a must read”
9. Protein Crystallography by T.L. Blundell and L. Johnson (January 28, 1976)
ISBN-10: 0121083500
“It is required reading for the scientist in the area of protein crystallography.”
10. Fundamentals of Crystallography edited by C. Giacovazzo (July 15, 2002)
ISBN-10: 0198509588
“A MUST HAVE for a lab!”
“For more advanced students Giacovazzo is a must.”

Short books that are quite useful for beginners are

- Introduction to Crystallography by Donald E. Sands (January 7, 1994)
ISBN-10: 0486678393
“A good addition to a practical methods course.”
- Crystallography Made Crystal Clear by: Gale Rhodes (February 16, 2006)
ISBN-10: 0125870736
“For the Novice/macromolecular user.”
- Crystal Structure Determination by: William Clegg (June 18, 1998)
“First time crystallographers should read this book.”
ISBN-10: 0198559011

For General X-ray Powder Diffraction

Introduction to X-Ray Powder Diffractometry by Ron Jenkins and Robert L. Snyder
(June 28, 1996)

ISBN-10: 0471513393

“A bit dated but still a good read.”

Elements of X-Ray Diffraction by B.D. Cullity and S.R. Stock (February 5, 2001)

ISBN-10: 0201610914

“This book is very inclusive on the subject of X-ray Diffraction.”

And finally a good book for SHELXL users is

Crystal Structure Refinement: A Crystallographer's Guide to SHELXL by Peter Muller,
Regine Herbst-Irmer, Anthony Spek, Thomas Schneider, Michael Sawaya (August 14,
2006)

ISBN-10: 0198570767

“Regine’s section on twinning is a marvelous!”

This list is certainly not all inclusive and is specific for X-ray diffraction and in particular to small molecule crystallography. This list should not be considered the only list the reader could consult. Every scientist is unique and will require their own personal library tailored to their needs. This list is a starting point to build or expand that library and to give the investigator the information they need to do their science.

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