ALLEN HUNTER'S YOUNGSTOWN STATE UNIVERSITY

X-RAY STRUCTURE ANALYSIS LAB MANUAL:

A BEGINNER'S INTRODUCTION[1]

OPTIMIZED FOR USE WITH SHELXTL AND DOS

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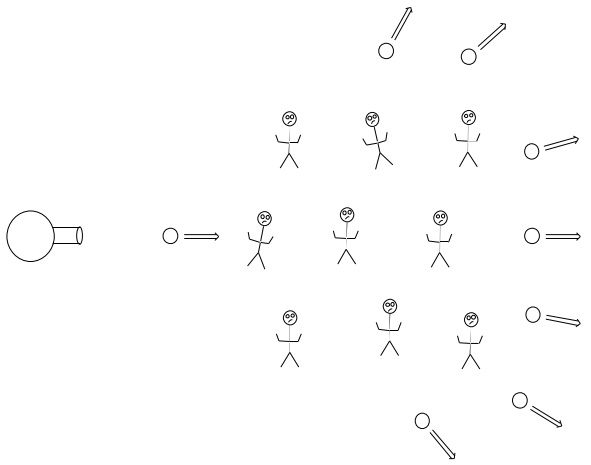
Detailed Comments On This Draft Manual Are Requested From All Users



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[1] This lab manual is based on the authors experience teaching crystallography to undergraduates and MS students at Youngstown State University, his experience with the software, the SHELXTL manual (Version 5.1) from Bruker AXS (Siemens), George Sheldrick's SHELX manuals, as well as the other references listed in the appendix.

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[7] Such "error messages" are most useful to me and will be more quickly incorporated into revised editions if they list the page, section, and line(s) of each error and suggestions for the correction of each.

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Suggestions for:

Improvements/Deletions/Additions/Changes (to Future Editions of this Manual)

I am writing this manual as a resource for the crystallographic educational community. I plan on improving future editions by incorporating feedback from manual users. This will be facilitated by the fact that it is being distributed as a .pdf file which will allow regular revision and rapid inexpensive distribution. For this to work, I need the user community to give me as much detailed feedback as possible. This could take the form of short notes to myself on any minor or major errors (and especially how to correct them!). I would also greatly appreciate longer sections of text that could be directly inserted into the main body or as separate appendices on topics not yet covered.

Known Problems With This Version of the Manual for Corrections in Future Editions:

1. The graphics is this .pdf file are at relatively low resolution because I have yet to find an acceptable way to get higher resolution graphics from XP (for DOS) into MS Word files, I welcome suggestions.
2. The list of teaching links is just starting, I need more suggestions.
3.

TABLE OF CONTENTS

[8] The diagram shown on the cover represents the thought experiment of bouncing quantum mechanical basket balls off of a team and using the resulting diffraction pattern to calculate the players' positions.

ACKNOWLEDGEMENTS

The author would like to gratefully acknowledge the contributions of the many people and organizations that have made the writing of this manual possible. I am a synthetic chemist who has learned sufficient crystallography to support my teaching and research but I do not have the expertise or experience to consider myself a professional crystallographer. However, I have been able to rely on substantial support, advice, and feedback from those more expert in crystallography than myself. I owe them a debt of gratitude for pointing out the errors in earlier editions of this manual and suggesting valuable additions and changes. I hope that they and others will continue to provide this invaluable service for this and future editions. I would particularly like thank the following individuals who have read over and made detailed comments and suggestions about this and earlier editions of this manuscript, especially: John Andrews, Rasika Dais, Jeanette Krause Bauer, Doug Powell, Zaki Sedge, Casey Raymond, and Tim Wagner. In addition, my Chemistry 832: Solid State Structural Methods students (especially Janet Gbur, Carrie Kolly, Mike Lufaso, Vince Lucarelli, and Jane Pollack) have provided me with invaluable feedback. I would also like to thank Bill Allen, John Jackson, Katy Landis, and Larry Curtin for providing crystals used to collect some of the diffraction data mentioned in this manual.

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PART I: GENERAL PROCEDURES FOR SOLVING STRUCTURES

CHAPTER XV. INDEX

It indexes the most important and/or commonly sought items in the manual, including: terms, concepts, commands, and symbols.

Dear Readers: Please feel free to suggest additional entries that should be added to this list.

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