ALLEN HUNTER'S YOUNGSTOWN STATE UNIVERSITY

X-RAY STRUCTURE ANALYSIS LAB MANUAL:

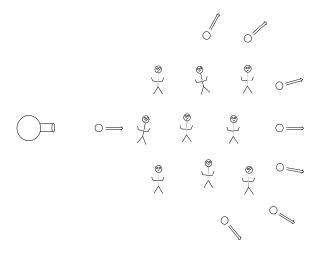
A BEGINNER'S INTRODUCTION¹

OPTIMIZED FOR USE WITH SHELXTL AND DOS

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<u>Detailed Comments On This Draft Manual Are Requested From All Users</u>



© Dr. Allen D. Hunter, March 24th 1997 and October 27th, 1998.

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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It is expected that this manual will undergo major updates at least once a year for the next several years with minor updates occurring more frequently.

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:

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

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.

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