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ALLEN HUNTER'S YOUNGSTOWN STATE UNIVERSITY

X-RAY STRUCTURE ANALYSIS LAB MANUAL:

A BEGINNER'S INTRODUCTION

OPTIMIZED FOR USE WITH SHELXTL AND DOS

Dr. Allen D. Hunter
Professor of Chemistry
Director of the YSU Structure Center
Department of Chemistry
Youngstown State University
1 University Plaza, Youngstown Ohio 44555-3663
adhunter@cc.ysu.edu
http://www.as.ysu.edu/~adhunter/index.html

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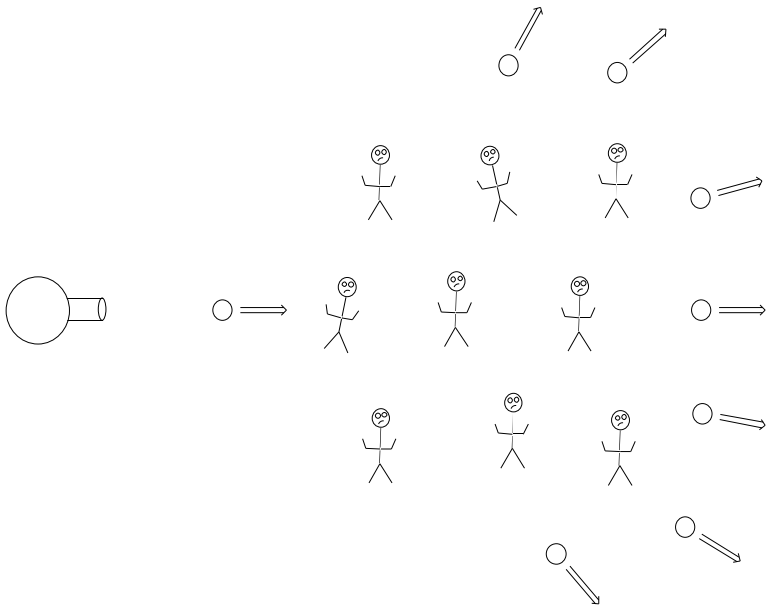
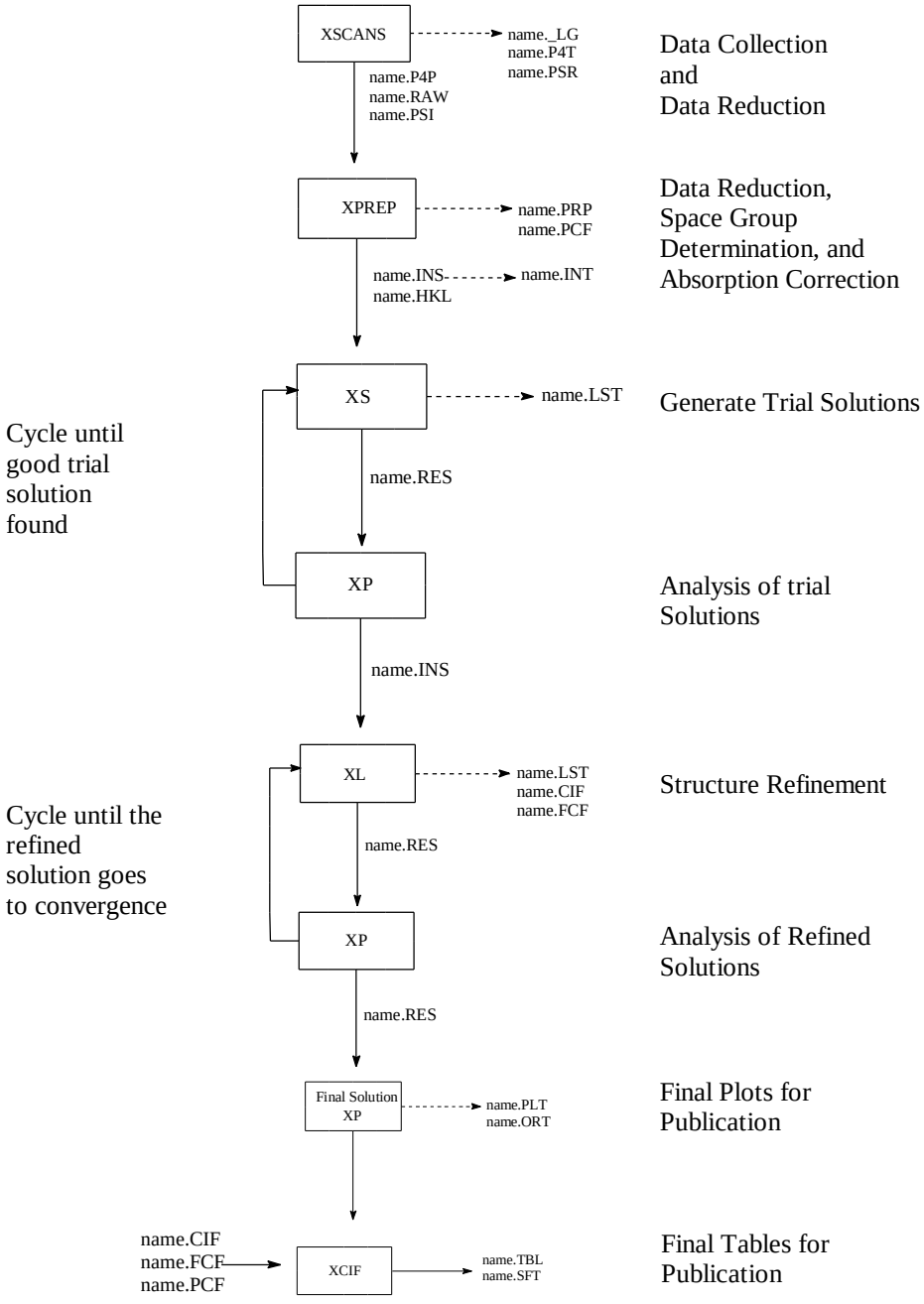
Detailed Comments On This Draft Manual Are Requested From All Users

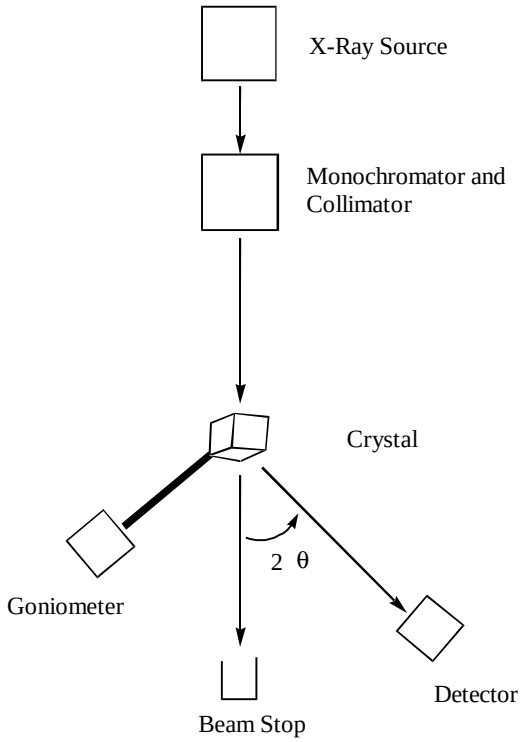


Flow Chart for a Typical Structure Solution



Chapters In This Text

Why X-Ray Diffraction Analysis for the Novice?



Single Crystal X-ray diffraction analysis is a technique whose practice has gotten dramatically easier over the last few years, whose power has increased tremendously, and whose cost per structure in terms of both dollars and person hours has dropped significantly. For these reasons, its use has been expanding rapidly from its former role as the tool of a few dedicated specialists to a tool that is accessible to anyone with a solid background in the sciences. Indeed, its use has expanded so far from its original homes in graduate inorganic and protein crystallography labs that all chemists, biochemists, biologists, physicists, geologists, medical researchers, and engineers should have a working knowledge of its use. To achieve this goal, it is essential that these people get their first exposure to crystallography as undergraduates. This will need to be done primarily by doing a much better job of integrating crystallography into our core undergraduate courses. In addition, student with the interest should be able to get a more in depth exposure in a solid state methods course in their senior year or as new graduate students. Both approaches to crystallography in the curriculum need to have strong laboratory experiences to go along with their lecture content. Indeed, the “hands on” experience of how crystallography is done is arguably more important than the formal lecture component. Fortunately, improvements in the cost of computers and ease of use of diffraction analysis software means that most of this “hands on” experience can take place in the typical departmental computer lab. The purpose of this lab manual is to provide students and instructors with a detailed step-by-step resource to help them in carrying out crystal structure analyses.