ORNL-6895

Chemical and Analytical Sciences Division

ORTEP-III: OAK RIDGE THERMAL ELLIPSOID PLOT PROGRAM FOR CRYSTAL STRUCTURE ILLUSTRATIONS

Michael N. Burnett
Carroll K. Johnson

Date Published: July 1996

Research sponsored by the
Laboratory Directed Research and Development Program

Prepared by the
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37831-6285
managed by
LOCKHEED MARTIN ENERGY RESEARCH CORP.
for the
U.S. DEPARTMENT OF ENERGY
under contract DE-AC05-96OR22464

CONTENTS

ACKNOWLEDGEMENTS vii

ABSTRACT ix

1. INTRODUCTION 1

1.1 WHAT IS ORTEP? 1
1.2 WHAT'S NEW IN ORTEP-III 2
1.2.1 User Interface 2
1.2.2 Screen Display 2
1.2.3 Output Formats 2
1.2.4 Color 2
1.2.5 Interactive Editor 2
1.2.6 Comments 3
1.2.7 Alternate Formats for Atomic Parameters 3
1.2.8 Atom "Features" 3
1.2.9 Critical Net Illustrations 3
1.2.10 Symmetry Operator Format 3
1.2.11 Miscellaneous Changes in ORTEP-III 4
1.3 REPORT ORGANIZATION 4

2. PROGRAMMING ORTEP 5

2.1 GENERAL PRINCIPLES 5
2.2 PROGRAMMING A NONSTEREOSCOPIC ILLUSTRATION FOR ORTEP . 10
2.2.1 Graphics Setup 10
2.2.2 Composing the Illustration 10
2.2.3 Drawing the Illustration 10
2.2.4 Terminating the Drawing of the Illustration 11
2.3 PROGRAMMING A STEREOSCOPIC ILLUSTRATION FOR ORTEP 11
2.3.1 Stereoscopic Rotations 11
2.3.2 Repeating a Sequence of Operations 12
2.4 DRAWING THE CUBANE STRUCTURE: AN EXAMPLE 12
2.4.1 Data Input for Cubane 13
2.4.2 Analysis of Structure 14
2.4.3 Programming the Cubane Illustration 14
2.4.4 Illustration of the Example 18

3. ORTEP INPUT 21

3.1 DEFINITIONS 21
3.1.1 Atom Designator Code (ADC) and Addressable Point 21
3.1.2 Vector Designator Code (VDC) 21
3.1.3 Atom Designator Run (ADR) 21
3.1.4 Atom Number Run (ANR) 22
3.1.5 Vector Search Code (VSC) 22
3.1.6 Sphere of Enclosure 23
3.1.7 Box of Enclosure 23

3.1.8 Reference, Working, and Standard Cartesian Coordinate Systems 23
3.1.9 Prime Parameters and Primer Constants 23
3.1.10 Atom Feature 24
3.1.11 Feature Number Run (FNR) 24
3.1.12 Number Run (NR) and Number Run Type 24
3.2 CRYSTAL STRUCTURE DATA INPUT 24
3.2.1 Title 24
3.2.2 Cell Parameters 24
3.2.3 Symmetry 25
3.2.4 Atom Parameters 27
3.3 INSTRUCTION INPUT 30
3.3.1 Instruction Format 30
3.3.2 Structure Analysis Instructions (100 Series) 32
3.3.3 Plotter Control Instructions (200 Series) 34
3.3.4 Drawing Parameter Instructions (300 Series) 35
3.3.5 ATOMS Array Instructions (400 Series) 37
3.3.6 Orienting Instructions (500 Series) 41
3.3.7 Positioning and Scaling Instructions (600 Series) 44
3.3.8 Atom Plotting Instructions (700 Series) 45
3.3.9 Bond Plotting Instructions (800 Series) 50
3.3.10 Label Plotting Instructions (900 Series) 53
3.3.11 Save Sequence Instructions (1100 Series) 55
3 3.12 Overlap Correction Instructions (1001, 821, 822) 56
3.3.13 Termination Instructions (Negative Series) 58
3.3.14 Supplementary Instructions 58
3.4 LIST OF FAULT INDICATORS 58

4. USING ORTEP-III 61

4.1 USER INTERFACE 61
4.2 SCREEN DISPLAY OF THE ORTEP ILLUSTRATION 62
4.3 PLOTTING THE ORTEP ILLUSTRATIONS 62
4.4 INTERACTIVE EDITOR 63
4.5 ALTERNATE FORMATS FOR ATOMIC PARAMETERS 64
4.6 ATOM “FEATURES” 65
4.7 MODIFYING ORTEP-III 67

5. TECHNICAL DETAILS 69

5.1 HOW ORTEP DRAWS ELLIPSOIDS 69
5.2 ELLIPSE RESOLUTION 71
5.3 HOW ORTEP DRAWS BONDS 72
5.4 OPTIMAL PARAMETERS FOR STEREOSCOPIC DRAWINGS 74

6. MATHEMATICS OF THERMAL-MOTION PROBABILITY ELLIPSOIDS 79

6.1 PROBABILITY DENSITY FUNCTION OF A TRIVARIATE NORMAL DISTRIBUTION 79
6.2 EQUIPROBABILITY ELLIPSOIDS 80
6.3 CHARACTERISTIC FUNCTION OF A TRIVARIATE NORMAL DISTRIBUTION 80
6.4 PRINCIPAL AXIS TRANSFORMATION 82

7. ORTEP EXAMPLES 85

7.1 CELL PACKING – 5-HYDROXY-5-PHENYLNORBORNANONE 85
7.2 HELICAL STRUCTURE – POLY-L-ALANINE 89
7.3 COORDINATION POLYHEDRA – POTASSIUM PERXENATE NONAHYDRATE 93
7.4 ATOM FEATURES – LYSOSOME MUTANT POLYPEPTIDE 96
7.5 CRITICAL NET – SODIUM CHLORIDE 100

REFERENCES 105

APPENDIX A — ORTEP-III SUBPROGRAMS 107

APPENDIX B — GLOSSARY OF VARIABLES IN ORTEP-III COMMONS 113

APPENDIX C — ORTEP-III FORTRAN SOURCE CODE LISTING 119

ACKNOWLEDGEMENTS

From previous versions of this report:[1,2]

We are particularly indebted to our colleagues, Drs. H. A. Levy, W. R. Busing, G. M. Brown, and R. D. Ellison for many helpful discussions and to R. A. Hollister, a summer participant with the ORNL Mathematics Division, who helped plan and code several parts of the initial 1965 release of the program. The initial draft version of ORTEP was written as a subroutine for the Busing, Martin, and Levy Function and Error Program, OR FFE; and many of the concepts and several of the subroutines of OR FFE are incorporated into the present program. Several parts of EIGEN were taken from a program written by R. E. Funderlic and B. Franz from the Central Data Processing group. Subroutine AXEQB was adapted from a subroutine obtained from the Oak Ridge Central Data Processing Library.

Additional acknowledgements:

We wish to thank Oak Ridge National Laboratory for providing computer resources for our ORTEP-III (and related crystallographic topology) World Wide Web pages at

http://www.ornl.gov/ortep/ortep.html

We especially thank Dr. Martin Kroeker for setting up a European World Wide Web site to mirror Oak Ridge's ORTEP-III web site at

http://tutor.oc.chemie.th-darmstadt.de/Ortep3/ortep.html

We thank all the people who have used ORTEP over the years and who have modified the program and made it available for others to use, including those listed at

http://www.ornl.gov/ortep/kin.html

A number of people assisted with the testing of ORTEP-III before the program was released to the public. It is impossible to list everyone here, but we appreciate all their efforts. We particularly thank: Dr. John Bollinger, Karl A. Byriel, Bjorn Dalhus, Dr. Bill Harrison, Dr. John C. Huffman, Prof. Gerald G. Johnson, Jr., Dr. Martin Kroeker, Dr. Anthony Linden, Dr. Wolfgang Poll, Dr. James V. Silverton, and Dr. Beverly R. Vincent.

We also thank Dr. Tim Pearson at the California Institute of Technology for the free graphics package PGPLOT, which enabled us to create one version of ORTEP-III that would produce screen graphics on a wide range of computer hardware. Thanks to Christian T. Dum and John S. Salmento for assistance with their ports of PGPLOT for DOS and Macintosh personal computers, respectively.

Thanks go to Kate Crennell for producing an executable version of ORTEP-III for Acorn microcomputers running the RISC OS operating system, which can be found at

http://micros.hensa.ac.uk/micros/arch-riscos.html

and again to Dr. Kroeker for making a PC LINUX version available at

ftp://tutor.oc.chemie.th-darmstadt.de/pub/ortep/linux/

ABSTRACT

This report describes a computer program for drawing crystal structure illustrations. Ball-and-stick type illustrations of a quality suitable for publication are produced with either spheres or thermal-motion probability ellipsoids on the atomic sites. The program can also produce stereoscopic pairs of illustrations which aid in the visualization of complex packing arrangements of atoms and thermal motion patterns. Interatomic distances, bond angles, and principal axes of thermal motion are also calculated to aid the structural study.