

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:<sup>1,2</sup>

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.

