1. INTRODUCTION

1.1 WHAT IS ORTEP?

Appropriate illustrations are essential in any manuscript dealing with crystallographic structures. An often quoted expression might justifiably be paraphrased to read that a well-planned figure is worth a thousand numbers. With the information explosion in the scientific literature, the author of a structure paper is obligated to provide the reader with “crystal clear” illustrations.

The Oak Ridge Thermal Ellipsoid Plot (ORTEP) program is a tool for drawing certain types of crystal structure illustrations. The program and the precision obtainable through machine plotting make feasible the production of detailed stereoscopic illustrations that are impractical to draw by conventional drafting methods. Several types of illustrations may be drawn with ORTEP. For a standard thermal motion drawing, an ellipsoid positioned on an atomic site represents a 3-D Gaussian probability density function showing the averaged atomic displacement as derived through the anisotropic temperature factor parameters for that atom. In critical net drawings, a very elongated or flattened ellipsoid of revolution, not positioned on an atomic center, represents the orientation of a saddle-point type critical point of the global density function. For simpler drawings of a crystal structure, all atoms are represented as spheres with sphere radii, or some other graphical variable, used to depict the chemical type of the atom. ORTEP cannot make van der Waal’s type drawings, which require overlapping spheres or ellipsoids.

Since its inception, four major goals have driven the development of ORTEP. These are listed here in decreasing order of their assigned importance. (1) The program must produce high quality illustrations, including stereoscopic pairs of thermal-motion figures, as free as possible of visually distracting approximations. (2) The program must be general both with respect to the types of illustrations it can draw and the types of computing and plotting equipment that it can utilize. (3) The program must be easy to use, require a minimum of input, and be easy to modify. (4) The computation time should be minimized. Since generality is placed higher in this goal list than ease of use, the program originally designed in the 1960s lacks several of the user-friendly attributes of the 1990s. However, the program seems to have survived the test of time better than some of its more user-friendly competitors. There were over 1000 citations of the 1965[1] and 1976[2] versions of the program in the 1995 Science Citation Index.[3] Since ORTEP has become widely used, we decided not to make changes that would render existing ORTEP input data sets inoperative.

ORTEP-III is written in device-independent FORTRAN, and the code should compile and run on any computer system that has a FORTRAN compiler. Compiled versions of ORTEP-III are available for DOS compatible and Macintosh† compatible personal computers. ORTEP-III is available on the World Wide Web at

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

or via anonymous ftp at ftp://ftp.ornl.gov/pub/ortep. Questions, comments, problems, suggestions, etc. may be sent via electronic mail to ortep@ornl.gov or via regular mail to either author of this report at P.O. Box 2008, Oak Ridge, TN 37831-6197, USA.

†Macintosh is a registered trademark of Apple Computer, Inc.

1.2 WHAT'S NEW IN ORTEP-III

For compatibility with existing ORTEP data sets, ORTEP-III retains ALL the functionality of OR TEP,[1] released in 1965, and OR TEP-II,[2] released in 1976. A brief description of the new capabilities in ORTEP-III is provided here. See the indicated sections of this report for more detailed information.

1.2.1 User Interface

ORTEP-III is a semi-interactive program that requests certain information from the user while the program executes. A default value for each item requested is provided in square brackets, and it will be used if the user simply hits the RETURN key (on some keyboards, the name of this key is ENTER). On systems that distinguish upper and lower case, care must be taken when entering file names to provide the correct case of the letters. (See 4.1.)

1.2.2 Screen Display

The screen drawing subroutines available in ORTEP-III use PGPLOT. PGPLOT is a free graphics library developed by T. J. Pearson at the California Institute of Technology. The package is written in FORTRAN and operates on a variety of platforms. Information about PGPLOT can be found on the World Wide Web at http://astro.caltech.edu/~tjp/pgplot or via e-mail to tjp@astro.caltech.edu. PGPLOT is **not** required to run ORTEP-III. The compiled versions of ORTEP-III for personal computers include the screen drawing capability. (See 4.2.)

1.2.3 Output Formats

Illustrations generated by ORTEP-III can be saved as Encapsulated Postscript™ or Hewlett-Packard Graphics Language (HPGL/2)™ files.† The files may be printed directly on a wide variety of printers and plotters or may be imported into a number of computer programs that accept these formats. (See 4.3.)

1.2.4 Color

By default, ORTEP-III plots its illustrations in black on a white background. The new 204 instruction allows color to be added to the illustrations if the output device supports color. Once a color is set, it remains in effect until another 204 instruction changes the color. A 204 with no parameter (or a "0") returns the plotting color to black (or pen #1). The screen and Postscript drivers built into ORTEP-III define color value 2 as red, 3 as green, 4 as blue, 5 as cyan, 6 as magenta, and 7 as yellow. (See 3.3.3.)

1.2.5 Interactive Editor

ORTEP-III provides a simple line editor for editing the input file without exiting the program. When the editor is invoked, the instruction set from the input file is displayed on the screen with line numbers (#) along with the editor commands shown below. (See 4.4.)

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†Encapsulated Postscript is a registered trademark of Adobe Systems, Inc. Hewlett-Packard Graphics Language Version 2 (HPGL/2) is a registered trademark of Hewlett-Packard Corporation.

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C=Change line #                   D=Delete line(s) # [#]
I=Insert line before #            T=Type line(s) [#] [#]
S=Save modified instruction set   O=Restore original instruction set
P=Save drawing as Postscript      H=Save drawing as HPGL
R=Redraw structure on screen      Q=Quit
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1.2.6 Comments

In previous versions of ORTEP, Format No. 3 trailer cards (see 3.3.1) were the only means of placing comments in the input file. This method still works in ORTEP-III, but a new method also exists. Among the ORTEP instructions, any line beginning with # is treated as a comment and is totally ignored by the program. Such comments can only go in the instruction portion of the input data and only at places where a new instruction could begin, i.e., comments cannot go between instructions and their trailer (continuation) cards. CAUTION: These comment lines are not printed in the ORTEP output file, and they are lost if the input file is edited with ORTEP-III's line editor.

1.2.7 Alternate Formats for Atomic Parameters

ORTEP-III provides a way to input atom parameters that are available in a "nonstandard" format. If the sentinel value (column 1) on the last symmetry card (see 3.2.3) in the ORTEP input file is "2" instead of "1", the program asks the user for the name of a file containing the atom parameters and branches to subroutine READIN to read the information. This subroutine may be recoded to read any desired format. (See 4.5.)

1.2.8 Atom "Features"

In earlier versions of ORTEP, atoms could be referenced only by their numeric positions in the input file; and atom number runs (ANR) (see 3.1.4) were used to select groups of atoms to be treated in the same manner. ORTEP-III allows two optional attributes called "features" to be included with each atom, and feature number runs (FNR) can be used to select groups of atoms having particular features. To handle features, a new parameter, number run type, has been added to the 100 series, 400 series, 505, 506, 700 series, 800 series, and 1001 instructions. Features should prove especially useful for polymeric materials such as proteins or nucleic acids and for critical net illustrations. (See 4.6.)

1.2.9 Critical Net Illustrations

ORTEP-III can produce critical net illustrations that depict some canonical topological characteristics of the global ensemble of overlapping atomic-thermal-motion Gaussian density functions in a crystal. (See 7.5.)

1.2.10 Symmetry Operator Format

The symmetry operators in the ORTEP input file (see 3.2.3) may now be provided in a free format using the xyz coordinate triplet notation found in the International Tables for Crystallography.[4] ORTEP is informed that this style for the symmetry operators is being used by having a "1" in column 1 of the cell parameter card (see 3.2.2). (A "0" or blank in that position indicates the old style is being used.)

Symmetry cards using this style do not have a specific format with the following two exceptions: (1) the symmetry information on each card must not go beyond column 72, and (2) column 1 must be blank on all symmetry cards other than the last one in the set, which must have a non-zero value in column 1. Below is an example set of symmetry cards to illustrate the flexibility of this style.

```
X,Y,Z
X   -Y   Z+1/2
X+0.5,  .5+Y,  Z
x+1/2,-y+1/2,1/2+z
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Letters may be either upper or lower case. Commas or spaces may be used to separate the components of the triplet. The three components may not have spaces within them. Decimal fractions may be used with or without an initial 0. Fractions may precede or follow the letters.

1.2.11 Miscellaneous Changes in ORTEP-III

- No longer provides a choice of centered symbols.
- Adds a parameter LOGC to the 100 and 400 series instructions to control the logic used (union or intersection) when multiple screening conditions are applied to the atoms. (See 3.1.5.)
- Makes the parameters on the Format No. 2 trailer cards of the 100 and 400 series instructions optional. (See 3.1.5.)
- Increases number of symmetry cards from 48 to 96. (See 3.2.3.)
- Increases number of atoms from 166 to 500. (See 3.2.4.)
- Makes entry of VDC_2 on Type 6 and Type 7 temperature factor cards optional. (See 3.2.4.2.)
- Increases number of Format No. 2 trailer cards per instruction from 10 to 20. (See 3.3.1.)
- Adds a 205 instruction to change the plotting pen width. (See 3.3.3.)
- Makes “no retrace” (instruction 303) the default. (See 3.3.4.3.)
- Adds a 304 instruction to control the resolution (smoothing) of the ellipsoids. (See 3.3.4.4.)
- Allows atom screening on the 403/413 and 404/414 instructions. (See 3.3.5.3.)
- Changes 600 instructions to allow input of SCAL2 or ellipsoid probability. (See 3.3.7.)
- Adds a 706/716 instruction to add another standard ellipsoid type (open octant football) for drawing atoms. (See 3.3.8.)
- Adds lower case letters for labeling. (See 3.3.10.)
- Centers titles automatically if they begin in column 1 of Format No. 3 trailer cards following instructions 902, 903, and 913. (See 3.3.10.)
- Makes instruction number 1001 an alias for the 511 instruction of OR TEP-II.[2] (See 3.3.12.)

1.3 REPORT ORGANIZATION

This report covers the following topics. First, Section 2.1 includes a summary table of the ORTEP instructions and is the part of the report to which the experienced user will routinely refer. The remainder of Section 2 provides an overview of how to program an ORTEP illustration, ending with a detailed example. Section 3 defines the terms used in this report and describes the ORTEP input in detail. Section 4 discusses the use of ORTEP-III in general terms while Section 5 looks at some of the more technical aspects. The mathematics of thermal-motion probability ellipsoids are described in Section 6. Lastly, several example structures illustrating a number of ORTEP’s capabilities are provided in Section 7. The appendices provide brief descriptions of the subprograms and the more important variables that are used in ORTEP along with a listing of the entire program’s FORTRAN code.