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An Interactive FORTRAN
Program for Crystal Structure
Illustrations

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Abstract

This report describes an interactive version of the ORTEP-2 program to draw crystal structure illustrations on a graphic display unit using the IBM/3277 Graphic Attachment Support under MVS(TSO). The program operation and plot-instruction input may be directed by menuing. Several file handling facilities have been introduced (i) in order to allow modifications of the crystal structure data, (ii) to repeat automatically added plot instructions with or without user control, and (iii) to provide a file tailoring for producing a hardcopy output on a mechanical plotter. Symmetry and lattice type input may be replaced by the related Hermann Mauguin space group symbol. Interactive positioning of atom labels, bond labels and explicit bonds is possible.

ORTEP-G Ein interaktives FORTRAN Programm zur graphischen Darstellung von Kristallstrukturen

Kurzfassung

Dieser Bericht beschreibt eine interaktive Version des ORTEP-2 Programms zur Darstellung von Kristallstrukturbildern auf einem graphischen Bildschirmgerät durch die Verwendung des IBM/3277 Graphics Attachment Support unter MVS(TSO). Die Steuerung des Programms und die Eingabe der Instruktionen zur Bildgestaltung wird mit Hilfe der Menütechnik vorgenommen. Spezielle Dateiverwaltungs-routinen wurden eingeführt, (i) um eine Korrektur der Kristallstrukturdaten zu ermöglichen, (ii) hinzugefügte Plot-Instruktionen automatisch mit oder ohne Benutzerkontrolle zu wiederholen und (iii) eine Ausgabe der erzeugten Bilder über einen mechanischen Plotter vorzusehen. Die Eingabe der Symmetrioperationen und des Gittertyps kann durch das zugeordnete Hermann Mauguin Raumgruppensymbol ersetzt werden. Atom- und Bindungsbeschriftungen und explizit hinzugefügte Bindungen können interaktiv in ihrer Ausgabeposition festgelegt werden.

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1. Introduction

The program ORTEP-G is, basically, an outgrowth of the XRAY/76 version/4/ of ORTEP-2/1,2,3/. This version has been modified to produce crystal structure illustrations in an interactive environment using a dual screen workstation concept, as described in more detail in section 2. The nucleus of the XRAY system has been implemented with minor changes. It provides general file handling capabilities, e.g. for reading the BDF, which is described elsewhere/4/. The BDF (Binary Data File) contains all basic information about a crystal structure and may also be used as input file for ORTEP-G.

ORTEP-G will draw thermal-motion probability ellipsoids at atomic sites and produce stereograms of a structure, including bond lengths and atom labelling in a number of optional configurations. A hidden-line feature is included in the program to omit the overlap between atoms and bonds. The composing of an illustration is realized by means of a variety of plot instruction codes. Especially, the symmetry operations may be replaced by the representing space group symbols. However, the basic philosophy of the ORTEP program has been retained. A number of features have been added. This includes a file tailoring for producing high quality plots on a mechanical plotter. A versatile file management has been provided for the handling of saved instruction sequences as defined by the interactive user even in the automatic mode of operation. Due to a refresh capability of the display monitor atom labels and bond length labels may be now (drawn correctly with respect to the original XRAY version) adjusted to a desired position on the screen. The cross hair cursor may be used to identify any atom by its name and internal code. Additionally, atoms or bonds may be colored, if an appropriate mechanical plotter is available.

The program is written in FORTRAN IV and is compiled with the IBM G1-compiler. An executable version of the program is currently implemented on the IBM/370-3033 configuration at the Kernforschungszentrum Karlsruhe(KfK). The IBM/3277 GAS PRPQ /5/ works under OS/VS2 MVS-TSO.

To minimize the core store requirement the program is organized in

an overlay structure (see App. C). A substantial fraction of the core requirement is caused by saved screens and an array size of 6000 full words needed for the correction of overlap. The size of the complete executable load module amounts to 300K Bytes. The plot routine supports XYNETICS, STATOS and VERSATEC plotters.

The CPU time depends upon the number of atoms involved in the illustration especially in a case of overlap correction. A screen picture is obtained in 1 minute typically. Under normal operating conditions in a multiprogramming environment the response time to most actions initiated by the user is of the order of 1 second.

Some definitions and conventions are described in section 3. The program operation is outlined in section 4. However, it should be mentioned, that some parts of this report are taken from /4/ with minor modifications due to the present mode of operation. A description of the program call is presented in section 5.

2. Execution with Interactive Graphics

The interactive mode of execution applies to both types of execution as outlined in section 4.2. All ORTEP cards are represented by panel definitions, so the user is able to enter the crystallographic data, control options and instructions, which together define an illustration, via the formatted alphanumeric screen of the IBM/3277 terminal. However, the user should be familiar with the cursor, joystick and keyboard features of the display units, which allow him to communicate with the program during execution.

2.1 Description of the Graphic Workstation

The ORTEP-G program uses the IBM/3277 Graphics Attachment Support Programming RPQ, which permits to attach a non-IBM graphic storage display monitor to the IBM/3277 Model 2 display terminal. In our case a TEKTRONIX 618 storage display unit has been used. For detailed

informations about this special approach to interactive graphics the user is referred to /5/. Both terminals are controlled by the so-called Dual Screen Manager (DSM). The basic functions of the DSM may be grouped into three categories:

1. Dual screen operations
2. Alphanumeric screen operations (on the IBM/3277)
3. Graphic screen operations (on the TEKTRONIX 618)

Communication between an application program and the dual screen workstation, as shown below in Fig. 1, is also realized by the DSM.

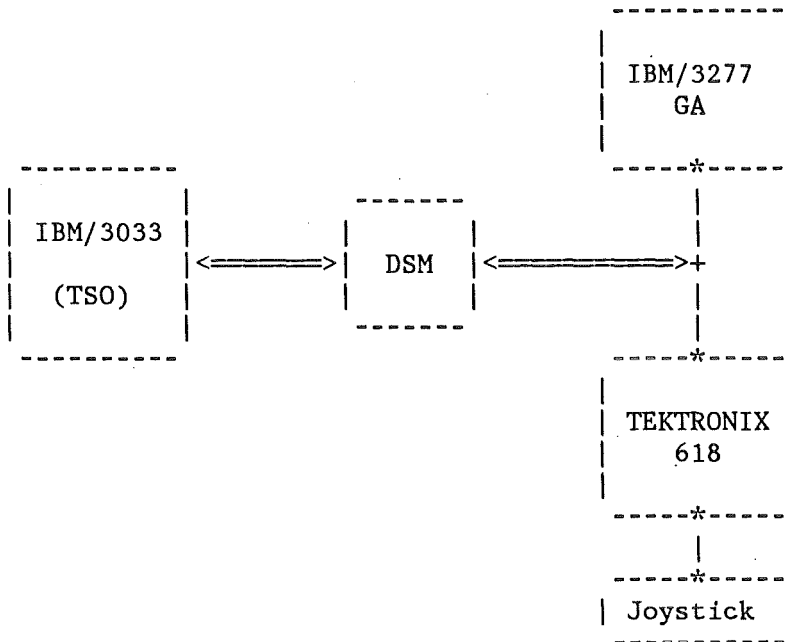


Fig. 1. Dual Screen Workstation

Wherein the alphanumeric screen may be used for function menuing, alphanumeric data entry and message prompting, all graphic data are displayed separately on the storage display TEKTRONIX 618 having intrinsic storage and refresh capability. For graphic input a cursor control joystick (crosshair cursor) is provided.

2.2 General Remarks on the Dialog Organization (Menus)

In this chapter some informations on the dialog organization are given. As already mentioned, each ORTEP input card (except XRAY specific cards) is now simply replaced by a panel definition thus taking advantage of the characteristics of the IBM/3277 display terminal in an interactive environment. The overall program operation will be directed by several user-defined panels, as given below:

1. Primary option menu
2. Instruction selection menu
3. Data entry panels (crystal structure data and instructions)
4. Program termination menu

A panel is generally a predefined screen image and may be a selection menu or a data entry display which prompts the user for input. Most of the panels related to crystal structure data and instructions are saved after completion for later use. The input for atomic parameters and temperature factors, for example, will be much easier, because a screen image previously saved may be restored on the screen including input data and cursor's position. Only those fields of a data entry panel must be overwritten, wherein changes of input data are necessary. The data are always retrieved from each input field of a screen definition, whether the user has modified it or not.

There are two types of function keys allowing the user to direct menu processing. The two (program access) PA keys on the keyboard are system-defined and may be not redefined by the program. They may be used in severe error situations (space overflow for graphic orders, etc.) only. Some of the (program function) PF keys are equated to application-defined operations.

All panels or menus prompt the user for any information, such as numerical data or text. In the following some remarks on performing input operations are given.

Data prompting is signaled by a cursor. The input operation is completed by pressing the ENTER key. The screen will be then updated and the input fields are highlighted in most cases. The cursor returns to the first entry line and additional changes are possible. If the user presses the ENTER key after each input line, the cursor is automatically moved to the next input line.

Once the user has entered all required information the END (PF3/15) key must be pressed to return to the higher level menu, if any, or to continue processing. The PF4 key serves to redisplay the screen image, if erased accidentally by the EOF key or any other interventions. The use of other function keys is explained where needed.

The type of input data in each panel depends on the specific ORTEP-G instruction. In case of trouble the user is referred to Appendix A.

For graphic input data the crosshair cursor should be moved to the desired position by means of the joystick. Any of the gray keys of the keyboard must be then pressed to complete the input operation.

3. Conventions and Definitions

3.1 Atom Designator Code (ADC)

Each atom position is specified as an 8-digit number *iii/jkl/nn* called the atom designator code (ADC). *iii* is the atom number in order of input, *jkl* are lattice translation digits along the cell edges with respect to an origin at 5,5,5, and *nn* is the symmetry number in order of input. Two ADC's (with a negative sign preceding the second) define a sequence of atoms including translations and symmetry operations. This is called an atom designator run (ADR). Thus 145502 -245603 would generate the 8-atom run 145502, 245502, 145503, 245503, 145602, 245602, 145603, 245603.

3.2 Atom Number Code (ANC)

The serial number of the atoms in the input atom list is called the atom number code (ANC). Two atom number codes represent a consecutive sequence of atoms. This is called an atom number run (ANR). Thus 4 8 specify atoms 4, 5, 6, 7 and 8 of the input list.

3.3 Vector Search Code (VSC)

Vector search codes consist basically of two ANR's and distances, which each place constraints on the search for interatomic vectors between atom sites. VSC's do not perform operations but are employed by instruction codes 101, 102, 402-407, 412-416, 511, 803-813 (detailed below) to limit vector searches. All VSC's which precede an instruction will act as a screen. This is in contrast to the original ORTEP program where the VSC cards follow the instruction cards. A maximum of ten (10) VSC's may be stored in the VSC array. If a vector does not satisfy the two ANR and DMIN-DMAX constraints of any VSC in the VSC array it is rejected.

4. General Description of Program Operation

This section describes the use of the interactive graphic computer program ORTEP-G.

4.1 Primary Option Menu

The first menu, which will be displayed after program start, is the primary option menu. The various ORTEP-G panels (used in that order) available to the user are shown in Fig. 2.

```
-----  
  
----- O R T E P   P R I M A R Y   O P T I O N   M E N U -----  
  
1 *CELL   PARAMETERS                10 *RADIUS TEMP. FACTOR FOR SPHER.  
2 *LATICE DEFINES CENTROSYM.,LAT.  11 *B     ISOTROPIC TEMP. FACTOR  
3 *SYMTY OPERATIONS (MAX. 96)      12 *U     ISOTROPIC TEMP. FACTOR  
4 *SPCGRP SPACE GROUP SYMBOL       13 *BIJ   ANISOTROPIC TEMP. FACTOR  
5 *ATOM   PARAMETERS ADD/REPLACE    14 *UIJ   RMS AMPLITUDE FOR BIJ  
6 *ATOMC  PARAMETERS IN CYL. C.     15 *BETA  ANISOTROPIC TEMP. FACTOR  
7 *ATOMD  DELETE ATOM ON THE BDF    16 *SEQ   PRECEDES EACH VSC OR INST  
8 *REPOSN CHANGE POSITION ON BDF     17 *INST  PLOT-INSTRUCTION MENU  
9 *RENAME CHANGE ATOM IDENT.       18 *VSC   VECTOR SEARCH CODES  
                                     19 *SYMBOL PLOT TITLE  
                                     20 *SVSTAR START OF SAVED SEQUENCE  
                                     21 *SVEND  END OF SAVED SEQUENCE  
                                     22 *SVEEXEC EXECUTION OF SAVED SEQ.  
                                     23  END    END OF INPUT FOR PLOT  
  
                                     24 EXEC   INITIALIZE NEW PLOT  
  
ENTER/VERIFY SELECTION NUMBER ==> _
```

* These operations are optional.

Fig. 2. Primary Option Menu

From this sequence the user selects an appropriate lower level menu or a data entry panel as needed by the ORTEP program. A successful application of the program for producing "optimized" illustrations should be possible especially for a routinely experienced user who is well acquainted with writing input cards for ORTEP-2. In the following some remarks on using the above options are given.

Each EXEC call (option 24) specifies a single plot and is followed by all optional instructions pertaining to that plot. After completion of the input on the EXEC panel the END option has to be used to "close" the current plot indicating that no further instructions are to be included. If all plot data are already given by the input file, these two above options are sufficient for drawing a plot. Confirming END on the termination selection menu, as described below in section 4.8, terminates the ORTEP-G run immediately, whereas a selection of option 24 initializes a completely new plot.

If an instruction needs alphanumeric information, it uses the last information that was read from the SYMBOL panel. If an instruction needs vector search codes, it uses the VSC's currently in that array. The maximum number of VSC's per array is ten. This procedure differs from the original version of ORTEP in which the alphanumeric information and vector search code cards were read after the instruction card that needed them.

All options related to crystal structure, such as CELL, LATIC, SYMTRY, SPCGRP, ATOM, ATOMC, B, U, BIJ, UIJ, BETA, RADIUS, ATOMD, RENAME and REPOSN must precede all SEQ, VSC, INST, SYMBOL, SVSTAR, SVEND and SVEXEC operations. In addition thermal parameters (if used) must immediately follow the atom parameters with the same atom label. To modify the generated instruction sequence in execution mode 0 the SEQ panel must be called first to change any INST or VSC input (see chapter 4.2.2).

The SVSTAR, SVEND and SVEXEC options may be used in the manual mode of execution only (see chapter 4.2.4).

In this version of ORTEP up to 96 equivalent positions may be entered. For higher symmetry spacegroups requiring 192 symmetry operations it is possible to operate either through the use of appropriate special positions or by expanding the input list of atoms to replace missing equivalent positions.

In this version of ORTEP up to 100 atoms may be entered. The atoms array (set up by 400 series instructions) of sites to be plotted, currently has a maximum of 500 atoms.

4.2 Modes of Execution

The user has the choice of two basic modes of operation. The first, and simplest mode, generates an instruction sequence according to the options specified on the EXEC panel. This mode of operation should be sufficient for most plotting requirements. If not, the user may use the second basic mode to specify the plot instructions explicitly. Details for applying these execution modes follow. The EXEC panel is given in Fig. 3.

```
-----  
----- O R T E P   EXEC - ENTRY PANEL -----  
  
ENTER/VERIFY LIST BELOW ==>  
  
INPUT (-1)/(0)/(1) FROM CARDS/F -1  MINIMUM BOND LENGTH (DMIN)      0.05  
EXECMODE (0)/(1) GENERATE INSTR. 0  MAXIMUM BOND LENGTH (DMAX)    2.00  
PLOTTYPE (0)/(1)/(2)/(3) INPUT  0  RADIUS OF STICK BOND          0.03  
OVERLAP (0)/(1) DO NOT CORRECT  0  ELLIPSOID PROBABILITY SCALE  0.00  
STEREO (0)/(1)/(2/3) DO NOT PLOT 0  X-DIMENSION OF PLOT IN INCHES 11.0  
PLOTAXES (1/2/3/4/5) X-Y AXES    0  Y-DIMENSION OF PLOT IN INCHES 11.0  
ELLIPSOID (1/2/3/4/5/6) ENV+OCT. 6  VIEW DISTANCE IN INC. (AUT.) 0.00  
H-ATOMS (1/2/3/4) IF EXECMODE=0  1  PLOT MARGIN=0.1*X-DIM./ATOM N 0.00  
SYMBOLS (0)/(1) DO NOT DRAW SYM. 0  ROTATION ABOUT X-AXIS IN DEG. 0.00  
CALC BLA (0)/(1) DO NOT CALC BLA 0  ROTATION ABOUT Y-AXIS IN DEG. 0.00  
DRAW BL (0)/(1) DO NOT DRAW BL   0  X-DISPLACEMENT OF ATOM SYMB.  0.90  
AUTOSCAL (0)/(1) DO NOT SUPPRESS 0  Y-DISPLACEMENT OF ATOM SYMB.  -0.50  
PRINT (0)/(1) DO NOT LIMIT A/B S 0  HEIGHT OF ATOM SYMBOLS (AUT.) 0.14  
BONDTYPE (-N)/(+N)                +3  PLOT SCALE USED IN./ANG.    1.00  
  
PRESS END (PF3) KEY TO RETURN TO THE PRIMARY OPTION MENU  
PRESS ENTER KEY TO READ IN THE DATA  
  
-----
```

Fig. 3. Data Entry Panel EXEC

Some of the variables are initialized with commonly used values. Normally, the values are taken from the input file FT05F001.

4.2.1 Execution Mode 0 Automatic Instruction Sequence

In this mode, a sequence of instructions is generated according to the following options, which may be set on the EXEC panel.

INPUT

directs the type of input to the ORTEP-G-program. For batch the complete input defining an illustration must be supplied from cards, or from a similar source (=1). Crystal structure data may be read in from XRAY-BDF (=0), or entered via the 3277 keyboard in the input fields provided on the 3277 screen (=1), or read in from a sequential file (=1) in mode 0. However, the crystal structure data are saved internally in the ORTEP-2-card format used for job submission (see chapter 4.7.3) or to avoid a repeated input of these data for a new EXEC.

PLOTTYPE

specifies the plotting of atoms at the input coordinates (=0), of atoms that form a single covalently-bonded molecule (n.b. also used for lattice or chain structures) (=1), of atoms that are enclosed by a single unit cell (including cell outline) (=2), or of atoms coordinated to a specified atom site (atom no. entered in line 8 at the right) within a specified radius (maximum bond length) (=3).

OVERLAP

indicates that the hidden line feature should be active (=1), or not (=0). Overlap correction can double computation times.

STEREO

specifies a single view (=0), a separated stereoscopic pair of drawings in black and white (=1) or a superimposed stereoscopic pair of drawings in red and green (red filter - left eye, green filter - right eye) (=2), or in red and blue (=3). The default stereo-rotation is +2.7 and -2.7 deg.

PLOTAXES

specifies the orientation of the plot axes, x (along the strip paper) and y (across the strip paper), with respect to the unit cell direc-

tions **a**, **b** and **c** (right-handed system is maintained).

ELLIPSOID

specifies the representation of each atom in the drawing -- as a point (=1), a spheroid of specified radius (=2), an ellipsoid envelope defined by the thermal motion parameters and the probability scale (=3), ellipsoid envelope with principal ellipses (=4), ellipsoid envelope with principal ellipses and axes (=5) and finally all the preceding features plus a shaded re-entrant octant of the ellipsoid facing the viewer (=6).

H-ATOMS

specifies how hydrogen atoms are to be treated in the plot (these are recognized in the input atom list by labels with a left-justified letter H). Hydrogens may be excluded completely (=1), included and sorted to the bottom of the atoms list (=2), included, sorted and plotted as spheroids with a radius of 0.1 Å (=3), or included in their order of input and handled identically to all other atoms (=4).

SYMBOLS

specifies if the atom labels are to be drawn on the plot (according to the x and y displacements and height) (=1), or excluded (=0).

CALC BLA

specifies the calculation of interatomic distances and angles, plus thermal eigenvalues and eigenvectors (=1), or not (=0).

DRAW BL

specifies the drawing of interatomic distance values on the plot adjacent to the stick bond.

AUTOSCAL

specifies the application of automatic scaling (=0), or not (=1). Automatic centering and contraction (by 0.9) is always applied. If the automatic scaling is suppressed the plot scale may be entered in the last line at the right, thus ensuring an identical scale for different plots.

PRINT

specifies that all lineprinter output is printed (=0), or limited to the headings and fault messages (=1).

BONDTYPE

is used in association with the maximum bond length and the radius of a stick bond. The bond-type, bond-max. and stick radius refer only to bonds between non-hydrogen atoms if H-ATOMS is set to 2 or 3.

The ellipsoid probability scale (SCAL2) enables the user to specify the ellipsoid size according to the thermal-motion probability.

probability (percent)	SCAL2	probability (percent)	SCAL2
10	0.76	60	1.72
20	1.00	70	1.91
30	1.19	80	2.15
40	1.37	90	2.50
50	1.54	99	3.37

Dimensions of the plot are specified in terms of the plot axes x (along the paper) and y (across). Stereoscopic plots automatically double the y dimension. In the interactive mode of operation these plot dimensions are also used to define the user address space (window). Depending on the type of display (stereo or not) a suitable viewport is set on the graphic screen.

Within these dimensions a plot margin is specified. This is used for drawing titles and explicit labels. The view distance is important for perspective drawings and may be automatically calculated by the program as 2.5 times the maximum x or y dimension.

The axial system specified by PLOTAXES may be rotated about the origin (automatically assigned in the 501 instruction according to the specified plottype) by specified amounts (positive values cause counter-clockwise rotation looking towards the origin).

When atom symbols are plotted, x and y displacements of the label centers with respect to the atom centers may be specified by the user. The height of the atom symbols is specified implicitly (where it is

taken as 0.01 times the two plot dimensions) or defined explicitly by the user. These parameters will be dependent on the type and size of the plot.

4.2.2 Modification of the Automatic Instruction Sequence

All the preceding information pertains to options on the EXEC panel, which are available under execution mode 0. However, it is possible, may be probable, that the more artistic (and adventurous) users will wish to invoke plot features not operable via the EXEC panel alone. If this is the case, the user has two choices either, to modify the automatic instruction sequence generated by execution mode 0, or to specify the entire instruction and control sequence under execution mode 1. Detailed information about the various types of instructions and options is given below.

The user may modify the automatic instruction sequence generated in execution mode 0 by calling the INST and/or VSC panels.

To change or insert any instruction the user has to select first the SEQ panel (Fig. 4) to specify the location in the automatic instruction sequence (each instr. is suitably numbered for this purpose) where an input instruction shall replace or precede an existing one.

To establish the position of the automatically generated instructions it is generally necessary (in a batch environment) to make a purely automatic run first. However, in this interactive mode of operation a list of all generated instructions will be displayed together with their internal sequence numbers immediately, so the user is able to select the correct position of the replaced or added instruction. The number and type of the generated instructions are caused by the information entered on the EXEC panel. In case of a replacement of a generated instruction the related data entry panel is called automatically. If an instruction must be inserted into the generated sequence, the instruction selection menu, as described in chapter 4.4 receives control.

----- O R T E P SEQ - ENTRY PANEL -----

LIST OF GENERATED INSTRUCTIONS :

1	211	7	604
2	301	8	611
3	303	9	705
4	401	10	802
5	407	11	902
6	501	12	202

DO YOU WANT TO CHANGE INST/VSC ==> inst
ENTER "PRECEDE" OR "REPLACE" ==> precede_

ENTER THE SEQUENCE NUMBER =====> (appears if the above requests
have been completed)

Fig. 4. Data Entry Panel SEQ

The VSC panel may be invoked from this panel whenever it is necessary to alter screening of vector searches for one or more instructions that need them. The VSC informations are stored in a separate array and are identified by their own serial numbers (also listed in the lineprinter output). Therefore VSC calls do not in any way change the instruction sequence but are used to replace (enter with matching serial no.), add to (enter with new serial no.) and delete (enter with matching serial no. but otherwise blank) existing VSC's in the array. First, the user is prompted to enter the serial number of that VSC array which should be changed or inserted. The related VSC information will be then displayed on the alphanumeric screen. After all desired data have been modified the ENTER key must be pressed to complete the input operation. Next, the user must press the END key to continue

processing via the primary option menu. The VSC panel is shown in Fig. 5.

```
-----  
----- O R T E P   V S C - E N T R Y P A N E L -----  
  
ENTER/VERFIFY LIST BELOW ==>  
  
SERIAL NUMBER IN THE VSC ARRAY           1  
  
ANC 1 (ORIGIN ANR)           - 1  
ANC 2 (ORIGIN ANR)           3  
ANC 3 (TARGET ANR)           1  
ANC 4 (TARGET ANR)           3  
BONDTYPE (-N)/+N)           3  
DMIN (ANGSTROMS)             0.05  
DMAX (ANGSTROMS)             2.0  
BOND RADIUS (ANGSTROMS)      0.03  
PERSPECTIVE BOND LABEL HEIGHT / -ANC1    0.0  
PERPENDICULAR DISPLACEMENT / ANC2      0.0  
NONPERSPECTIVE LABEL HEIGHT / PH. DMIN   0.0  
PERPENDICULAR DISPLACEMENT / PH. DMAX   0.0  
-1/0/1 FOR 1/2/3 DECIMAL PLACES        0.0  
PEN COLOR FOR BOND (1/2/3/4)           1.0  
  
PRESS END (PF3) KEY TO RETURN TO THE PRIMARY OPTION MENU  
PRESS ENTER KEY TO READ IN THE DATA
```

Fig. 5. Data Entry Panel VSC

Each call of a VSC panel must be preceded by a SEQ operation which specifies the location within the generated instruction sequence, where the VSC array is to be updated. In this way the VSC's can be 'synchronized' with the specific instructions that use them. Users will find that careful use of the VSC and INST operations in the automatic execution mode is powerful medicine indeed.

4.2.3 Repeating a Sequence of Added Instructions

Necessary plot instructions pertaining to an illustration are normally determined only through the EXEC panel. However, in many cases it is desirable to enlarge the atom list with distinct elements in an out-of-cell position. Especially when drawing atom or bond labels, it is burdensome for a series of plots to redefine again and again new or changed instructions as outlined in the previous chapter. This is especially true in a most common case concerning stereo plots.

Additionally, if many screens have to be saved, the internal core may be not sufficient and in some situations it is almost impossible to handle very complex illustrations. Therefore, an algorithm has been developed to repeat automatically additional instructions for any kind of plot. Such instructions are placed into a so-called **instruction lookaside buffer**, because saved instructions should be executed during a next EXEC without user intervention. This buffer file defined by the FORTRAN file definition statement FT34F001 is sequentially organized and may contain SEQ, INST or SYMBOL cards according to the ORTEP card format. Further instructions may be included.

However, for updating purposes the buffer file management must perform the following operations:

1. If possible, fill the buffer from input file FT05F001
2. Update the buffer with new instructions after an EXEC
3. Open the buffer (makes the entries available for access)
4. Determination of the order in which currently added instructions must be executed with respect to a saved instruction.

First it has to be checked, if there are any instructions in the input data set that have to be transferred to the instruction lookaside buffer. Otherwise the stack is empty. Before executing a generated instruction, it has to be checked each time, if the buffer contains an instruction that should be run first or not. The same procedure applies to those instructions which are defined additionally and which are stored in the sequential file FT33F001 together with the current EXEC card.

Externally defined instructions are executed first. Whenever an instruction of the buffer is executed, they are executed from top to bottom.

If the drawing of an illustration has been finished, all instructions are automatically merged to the buffer using an external sort algorithm assumed that not both files (FT33F001 and FT34F001) are empty. Otherwise a normal copy step is used.

----- O R T E P INST LOOKASIDE BUFFER MANAGEMENT PANEL -----

ENTER/VERIFY OPTION ==> C

CURRENT INSTRUCTION FILE IS EMPTY⁺

- R - RESET INST LOOKASIDE BUFFER TO INPUT
- D - DELETE CURRENT INSTRUCTION FILE
- M - MERGE CURRENT INSTRUCTION FILE AND INST LOOKASIDE BUFFER
- C - COPY CURRENT INSTRUCTION FILE TO INST LOOKASIDE BUFFER
- N - RENUMBERING OF SEQUENCE NUMBERS FORCED FOR THE NEXT EXEC
- S - SAVE ALL (BACK UP) ALL INSTRUCTIONS

PRESS END (PF3) KEY TO RETURN TO THE PRIMARY OPTION MENU
PRESS ENTER KEY TO READ IN THE DATA

+ Message written after completion of the selected option

Fig. 6. Instruction Lookaside Buffer Management Menu

Furthermore, this automatic update of the instruction lookaside buffer may be directed by the interactive user by calling the buffer management panel as shown in Fig. 6 from the program termination menu (see chapter 4.7 and 5.2). However, a more detailed description of the working of the buffer routines and their embedding in the ORTEP pro-

gram will not be given here.

----- O R T E P RENUM - ENTRY PANEL -----

LIST OF GENERATED INSTRUCTIONS :

1	211	7	604
2	301	8	611
3	303	9	705
4	401	10	802
5	407	11	902
6	501	12	202

CONTENT OF THE INSTR. LOOKASIDE BUFFER

11 901

IF ANY SEQUENCE NUMBERS ARE TO BE CHANGED,
MOVE THE CURSOR TO THAT LINE, PRESS ENTER
AND THE PF1 KEY, ELSE PRESS THE PF3 KEY

Fig. 7. Data Entry Panel RENUM

In some cases, the sequence number of any saved instruction must be reset to a new one after another choice on the EXEC panel (if not, the same instructions were generated), because some instructions may be executed only in a distinct order. Otherwise, if there is only a "small" change of the sequence numbers and does not matter in the execution sequence, such a renumbering is not necessary. For an experienced ORTEP user, this decision will not become a problem. On the other hand, a related panel may be called from the panel as given above in Fig. 7.

4.2.4 Execution Mode 1 Manual Instruction Sequence

Those users who have read and tried the preceding automatic options and find the plot lacking, ORTEP-G retains the original ORTEP procedure where all instructions are entered on cards (structure parameters may still be read from the BDF , though) or, in our case, from panels. This mode of operation is undoubtedly the most flexible and will allow the user to plot a drawing with an almost infinite range of options. To do this, however, the user should be familiar himself with the function and format of most control and instruction cards (72 varieties) described below. This is no small task and it may be necessary for the user to refer to the more detailed ORTEP report and revisions /1,2,3/. Nevertheless there are a few basic rules for sequencing that may be summarized as follows:

- (1) Vector search codes (VSC) must be defined before the instructions that use them.
- (2) The instructions should appear in approximate ascending order of their codes, except for INST 503 and 511 which must follow all other 500 and 600 series instructions, and precede all 700 and 800 series instructions.
- (2) Parts of the instruction sequence may be saved by inserting SVSTAR (start saving instructions) and SVEND (finish saving instructions) cards at appropriate places. The saved instructions may be then subsequently re-entered into the sequence using SVEXEC. This is a useful feature for stereo plots.

4.3 Crystal Structure Data Input

The crystallographic structure data may be grouped into the following categories:

1. Cell dimensions
2. Symmetry center and Bravais lattice type
3. Equivalent point positions
4. Atomic parameters

The input of the lattice type and symmetry operations may be simplified in some cases by entering the related space group symbol. The atomic parameters pertain to the atomic positions and temperature factors.

Structure parameters may be entered from different sources of input. If all relevant information is given on the FORTRAN file FT05F001, the appropriate ORTEP cards are then extracted from it and transferred to the file FT32F001. Depending on the input mode on the EXEC panel, these parameters may also be received from several panels on the primary option menu. In each case, a record according to the ORTEP input format has been written on the file FT32F001 which is then used for all following plots without need to redefine all data on the screen. With respect to the interactive mode of operation and to a batch processing environment respectively, the user has the possibility to gather the crystal structure data

- A. from the binary data file on NTAPEA and cards (batch only)
- B. from the binary data file on NTAPEA and panels
- C. from CRT via the primary option menu
- D. from cards (internally saved or in batch)

How to write input cards the user is referred to Appendix A. Usually structure parameters will be extracted exclusively from NTAPEA and modified if necessary with a few well-chosen operations (e.g. RENAME, ATOM, ATOMD, REPOSN, etc.).

4.3.1 Cell Dimensions

The cell parameters may be entered either all in direct space or

refer to the reciprocal unit cell. The angles may be supplied as either cosines or in degrees.

4.3.2 Symmetry Center and Bravais Lattice Type

One must supply separately whether the cell is centric or acentric. The lattice type may be entered using one of the following symbols:

P	primitive
I	body centered
R	rhombohedral
F	face centered
A	a centered
B	b centered
C	c centered

Note, that P is used for rhombohedral space groups indexed as rhombohedral and R is used for rhombohedral space groups indexed as hexagonal. In the centric case with the origin at the center of symmetry, only those operations not involving the center should be supplied.

In the trigonal case one must give for P-space groups the hexagonal lattice constants and the lattice type P; for R-space groups the standard setting will be assumed for a hexagonal cell, wherein a,b,c must be given explicitly on the CELL panel for a rhombohedral cell and lattice type P.

4.3.3 Equivalent Point Positions

The symmetry of the space group is indicated by supplying a set of general equivalent positions. A simple rule is that any general equivalent position in the international tables may be written verbatim with conventions as explained in Appendix A. The identity (x,y,z) is always expected and must be given. The symmetry data supplied are transformed into a set of rotation matrices and translation vectors to generate equivalent positions in direct space.

4.3.4 Space Group Symbols

The space group of the crystal structure may be defined by the related Hermann Mauguin symbol, which is analysed by a special program/6/ to yield all necessary symmetry and lattice type information. A list of all allowed space group symbols is given in Appendix E.

4.3.5 Atomic Parameters

These parameters pertain to positional parameters for each input atom and to anisotropic temperature factors. The latter must be entered on individual panels (options 10 to 15 on the primary option menu) after each related atom input. However, isotropic temperature factors may be supplied on the ATOM panel. Fig. 8 shows the ATOM data entry panel.

```
-----  
  
----- O R T E P   A T O M - E N T R Y   P A N E L -----  
  
ENTER/VERIFY LIST BELOW ==>  
  
A T O M   I D E N T I F I C A T I O N   =====> _  
X C O O R D I N A T E  
Y C O O R D I N A T E  
Z C O O R D I N A T E  
I S O T R O P I C   T E M P E R A T U R E   F A C T O R  
C O O R D I N A T E   S Y S T E M   D E S I G N A T O R  
  
P R E S S   E N D   ( P F 3 )   K E Y   T O   R E T U R N   T O   T H E   P R I M A R Y   O P T I O N   M E N U  
P R E S S   E N T E R   K E Y   T O   R E A D   I N   T H E   D A T A  
  
-----
```

Fig. 8. Data Entry Panel ATOM

Several input alternatives are possible for the positional and temperature parameters.

4.3.6 Modification of the Crystallographic Input Data

For an improved flexibility of the interactive program an algorithm has been developed to modify some data of the actual crystal structure.

----- O R T E P CRYSTAL STRUCTURE DATA OPTION MENU -----

1	CELL	PARAMETERS	10	RADIUS	TEMP. FACTOR FOR SPHER.
2	LATICE	DEFINES CENTROSYM.,LAT.	11	B	ISOTROPIC TEMP. FACTOR
3	SYMTY	OPERATIONS (MAX. 96)	12	U	ISOTROPIC TEMP. FACTOR
4	SPCGRP	SPACE GROUP SYMBOL	13	BIJ	ANISOTROPIC TEMP. FACTOR
5	ATOM	PARAMETERS ADD/REPLACE	14	UIJ	RMS AMPLITUDE FOR BIJ
6	ATOMC	PARAMETERS IN CYL. C.	15	BETA	ANISOTROPIC TEMP. FACTOR
7	ATOMD	DELETE ATOM ON THE BDF			
8	REPOSN	CHANGE POSITION ON BDF			
9	RENAME	CHANGE ATOM IDENT.			

PRESS END (PF3) KEY TO END
PRESS ENTER KEY TO READ DATA AND DISPLAY

ENTER NUMBER OF DESIRED OPTION ==> _

Fig. 9. Modify Frame for Crystal Structure Data

As already mentioned above, all crystallographic data are accumulated on file FT32F001. If the user has selected a desired option, the related panel will be then displayed with the current data assumed

that an appropriate "card" exists on the input file. For atom input the user is requested to enter the ANC of the desired atom. If the atom is not given in the input list, i.e. to add an atom, then a number greater than the last ANC in the list must be entered. It should be mentioned, that atom input and anisotropic temperature factors must be modified pairwise. After completion of all input operations pertaining to the selected option the file FT32F001 is always updated using the file FT35F001 as temporary storage.

4.4 Instruction Input (INST)

The user may direct the plotting through the use of specific instruction codes (INST) and vector search codes (VSC). A brief description of the present instruction codes is given below. For writing input cards the user is referred to Appendix A, where additional remarks on using an instruction code are included. To add a plot instruction the user must enter the specific instruction number on the INST selection menu, as given in Fig. 10.

----- O R T E P INST - SELECTION MENU -----

ENTER INSTRUCTION CODE BELOW =====>

STRUCTURE ANALYSIS	(101,102,105,106)	:
THERMAL EIGENVECTORS	(103)	:
PLOTTER/CRT CONTROL	(201-204,211)	:
PLOT BOUNDARY	(301-303)	:
EXPLICIT UPDATE OF ATOMS ARRAY	(401,411)	:
UPDATE ATOMS ARRAY	(402-407,412-416)	:
CLEAR ATOMS ARRAY	(410)	:
PLOT ORIENTATION - definition -	(501)	:
PLOT ORIENTATION - rotation -	(502,503)	:
OVERLAP CORECTION	(511)	:
POSITION AND SCALING	(601-604,611-613)	:
ATOM PLOTTING	(701-704,711-714)	:
COMPOUND ELLIPSOID	(705,715)	:
700 SERIES CONTINUE	(701-715)	:
EXPLICIT STICK BONDS	(801,811)	:
BOND PLOTTING	(802,803,812,813)	:
LABELS	(901-906,908,909,913-916)	:915_
CONTINUE FOR CENTERED SYMBOLS	(908,909)	:

PRESS END (PF3) KEY TO RETURN TO THE PRIMARY OPTION MENU
PRESS ENTER KEY TO COMPLETE INPUT AND TO CALL THE INSTRUCTION SUBMENU

Fig. 10. Instruction Selection Menu

This menu will be re-displayed upon exit from an instruction sub-menu. The PF3 key must be pressed, as indicated, to return to the primary option menu. The current plot may be now closed using the END option (23) or further instructions may be changed or inserted by invoking the SEQ panel (option 16).

4.4.1 Structure Analysis Instructions (100 Series)

These instructions are used to calculate bond distances and angles, and principal axes of thermal motion. INST 101 calculates bond distances within the DMAX sphere from origin atoms described by an ADR, to target atoms defined by an ANR, and according to preceding VSC parameters. INST 102 is equivalent to 101 but also calculates angles. INST 103 calculates the thermal eigenvectors and eigenvalues for all input atoms. INST 105 is equivalent to 101, except that only those atom sites already present in the atoms array (usually via 400 series instructions) are eligible as origin sites for the DMAX spheres. INST 106 is equivalent to 105 except that the search is iterated so that every new atom found by the search becomes an origin site (provided it is within the specified ADR/ANR and VSC constraints).

4.4.2 Plotter/Display Control Instructions (200 Series)

INST 201 and INST 211 serve for initialization of the plotter or CRT, respectively. In case of a stereoscopic representation appropriate viewports are defined for the graphic screen. INST 204 allows the user to change the color of up to three atoms (given by their ANC), if the XYNETICS plotter is used for plot output. Bond coloring is realized via the VSC panel.

4.4.3 Plot Boundary Instructions (300 Series)

These instructions specify the plot dimensions, viewing distance, general lettering orientation, and line retracing. INST 301 defines the plot boundaries, plot margins and perspective viewing distance.

INST 302 rotates regular titles and chemical symbols counter-clockwise from the plotter x axis by a specified angle. INST 303 retraces certain lines by a specified displacement to enhance the perspective and clarity.

4.4.4 Atoms Array Instructions (400/410 Series)

This series is used to specify which atomic sites are to be included in the illustration. Groups of sites are added to or eliminated from the atoms array by the 400 series and 410 series instructions, respectively. Duplicate entries of the same atomic position are prevented by the program. INST 401/411 adds/subtracts sites to/from the atoms array according to the explicitly specified ADC's. Before enlarging the atoms array in a next plot the user may use the identify-option of the termination selection menu to find the sites to be added. INST 402/412 adds/subtracts to/from the atoms array atom sites within the target ANR which occupy sites within DMAX of sites defined by the origin ADR. If the origin ADR atoms are also to be added/subtracted to/ from the atom array their atom numbers must be within the specified target ANR. INST 403/413 adds/subtracts target atoms(defined by ANR) which are within an orthogonal box (parallel to base vectors of the reference cartesian system) centered about each origin atom (defined by ADR). INST 404/414 is identical to 403/413, except a triclinic box of enclosure (defined by cell axes) is used. INST 405/415 adds/subtracts atom sites to/from the atoms array by searching for all target atoms (defined by ANR) within convoluting spheres of enclosure at all sites placed in the atoms array by previous 400 series instructions (within the specified ADR/ANR and VSC instructions constraints). An important use of INST 405 is to complete the coordination shells around metal atom clusters without having to describe any of the atoms individually. The INST 406/416 is similar to 405/415, except that the newly added atoms are also eligible as origin ADC's. DMAX must be chosen judiciously with this instruction so that the search does not cross molecular boundaries. INST 407 is an XRAY-exclusive which is identical to 406, except that a site generated by the iterative search that is related by pure cell translations to a site already existing in the atoms array, is ignored. This is useful for drawing an infinite chain

molecule. INST 410 clears the atom array.

4.4.5 Orienting Instructions (500 Series)

These instructions are used to orient the reference and working cartesian axial systems. The reference system is used for all internal operations, except plotting where the working system is used. INST 501 specifies the reference cartesian system in terms of an origin (one ADC) and two vectors, v_1 and v_2 (two ADC's each). The plotter ortho-normal axial system may be specified by (\cdot = vector product)

-type A with $x = v_1$, $y = v_1 \cdot v_2$, $z = v_1 \cdot (v_1 \cdot v_2)$,

or,

-type B with $x = v_1$, $y = (v_1 \cdot v_2) \cdot v_1$, $z = v_1 \cdot v_2$.

INST 502 rotates the reference system axes. Numbers 1, 2 or 3 indicate rotation about the x, y or z axes for the specified angles (positive degrees for counter-clockwise rotation looking down the axis towards the origin). INST 503 rotates the working axial system about one axis of the reference system. INST 503 normally precedes each member of a stereoscopic pair of plots. The working and reference axial systems are made coincident for INST 501 and INST 502.

4.4.6 Positioning and Scaling Instructions (600/610 Series)

These instructions are used to position, center and scale the drawing. INST 601 explicitly specifies the origin of the reference axial system and the scales of the coordinates (SCAL1) and temperature factors (SCAL2). INST 602 is equivalent to 601, except the coordinates are automatically scaled. INST 603 is equivalent to 601, except the plot is automatically centered. INST 604 automatically scales and centers the coordinates within the plot boundary. INST 611, 612 and 613 are equivalent to INST 601, 602, and 603 except that they specify origin increments and scale products. These instructions are used to shift, contract or expand the plot. In all the 600 series instructions the thermal ellipsoid probability scale (SCAL2) has a default value of

1.54 (50 percent).

4.4.7 Atom Plotting Instructions (700/710 Series)

These instructions plot atoms stored in the atoms array, unless outside a specified ANR. Different combinations of principal ellipses, ellipsoid envelopes, eigenvector axes and octants are optionally drawn with the 700 series instructions. INST 701 generates an ellipsoid with principal ellipses and octant shading. INST 702 draws principal and enveloping ellipses without axes. INST 703 provides an open model with principal ellipses and axes. INST 704 draws the enveloping ellipse only. INST 705 enables a combination of components.

Chemical symbols are also drawn with these instructions, symbol height, parallel and perpendicular offset should be supplied to position label written relative to the atom center. To position each symbol individually, the 900 series instructions may be used interactively. The thickness of the boundary ellipse may also be varied as a function of plot height (A0 is the increase in radial dimension added to the width of the original line, and A1 is the rate of increase in radial dimension with height). INST 711-715 are identical to INST 701-705, except that the lineprinter output is limited.

4.4.8 Bond Plotting Instructions (800/810 Series)

These instructions draw interatomic bonds and contacts, and values of bond lengths. 800 series instructions use VSC's stored in the VSC array to specify the search constraints for bonds between sites in the atoms array. For a more thorough description the user is referred to /3/. INST 801 draws only bonds which are explicitly specified by pairs of ANC's. For an improved interactivity this instruction has been rewritten to draw one bond at a time only. Bond type and bond-distance label parameters must now be defined on this panel. INST 802 draws stick bonds between atoms in the atoms array according to the preceding VSC's. INST 803 is equivalent to 802, except that it draws line bonds between symbols centered on the atom sites.

4.4.9 Label Plotting Instructions (900/910 Series)

These instructions draw titles or labels which have been previously specified on a SYMBOL panel (see below) in terms of the height of the symbols and the position for the label center (rotation of titles is done by INST 302). INST 901 draws chemical symbols for specified atoms (in terms of ANC's). INST 902 draws a general title specified on a SYMBOL panel. INST 903 is equivalent to 902, except that the label base is aligned with the vector between the two specified ADC's. INST 904/905/906 draws bond length values along the bond vectors to 1/2/3 decimal places, respectively. INST 908 and 909 draw centered CALCOMP symbols (symbol numbers 0-14). The former with pen up while moving to the symbol position, the latter with pen down. INST 911-916 are equivalent to 901-906, except the titles and labels are drawn in perspective.

In the interactive mode the atoms or bonds to be labeled may be selected by using the crosshair cursor, which appears on the graphic screen. The user is prompted to move this cursor to the atom (or two atoms in turns, if a bond should be labeled) and to press any gray key of the alphanumeric keyboard of the 3277. The ADC's are then transferred into the related input fields. After completion the pressing of the ENTER key initiates drawing the label at the desired location. However, because the label (for an atom or bond) is written in the refresh mode, any changes to the offset and height of the label causes the old label to be erased and then to be drawn at the new position in turns. Fig.11 shows the entry panel for the instruction 915 after completion.

To fix a label at a desired position, the user must press the PF1 key. Then the label will be redrawn in the stored mode, i.e. it is discarded and may not be removed from the screen. In order to place another label, pressing of the PF5 key leads the cross hair cursor to be redisplayed, so the user is able to select a further atom or bond for labelling. The same procedure may be performed for positioning titles on the screen. In this case an additional input field is pro-

vided on this panel. For each fixed label or title a pair of SEQ/INST cards preceded by a SYMBOL card, where needed, is saved on the file FT33F001 for later use. By changing the positional parameters many "titles" may be placed on the screen, if desired.

----- O R T E P INST - 915 ENTRY PANEL -----

ENTER/VERIFY LIST BELOW ==>

CONTINUATION CODE ==> _0
ADC 1 (LABEL ADR) 356510.
ADC 2 (LABEL ADR) 156510.
X EDGE RESET (INCHES) 0.0
Y EDGE RESET (INCHES) 0.0
LETTERING HEIGHT 0.14
PARALLEL OFFSET 0.2
PERPENDICULAR OFFSET 0.2

PRESS END (PF3) KEY TO END
PRESS ENTER KEY TO READ DATA AND DISPLAY
PRESS REPEAT (PF5) KEY FOR A NEXT LABEL
PRESS SAVE (PF1) KEY TO FIX THE LABEL

Fig. 11. Data Entry Panel for a 900 Series Instruction

4.5 Special Instructions

4.5.1 Overlap correction (511)

INST 511 eliminates the overlap of atoms and bonds from the drawing. This feature requires up to 2 times the computing time of non-corrected drawings. INST 511 must follow all other 500 and 600 series instructions and precede all 700 and 800 series instructions. Bonds are included according to the VSC array, similar to the 800 series instructions.

4.5.2 Plot Title

The alphanumeric information used by the 900 instruction series may be entered from the SYMBOL panel. For correct centering on plot this information should be centered on the line. Each SYMBOL panel must be called before a 900 series instruction which uses it. In the automatic mode the TITLE card replaces the text as specified on the SYMBOL panel.

4.5.3 Saved Sequence Instructions

As already mentioned, it is generally not necessary to use this feature, because in most cases the automatic mode of operation together with the instruction lookaside buffer management is sufficient to produce a complex illustration (see also chapter 4.2.3 and 4.2.4). The SVSTAR operation specifies that the following instruction and control cards (as saved internally) are to be saved on the scratch file NTAPEE. The SVEND switches off the save process and rewinds the scratch file. The SVEEXEC causes the instructions saved on NTAPEE via the SVSTAR and SVEND, to be inserted into the instruction sequence at its point of entry.

4.6 Terminating the Drawing of an Illustration

If all instructions for an illustration have been entered the drawing must be completed by the selection of the END OF INPUT option (23) on the primary option menu.

4.7 Program Termination Menu

After completion of an illustration the program returns to the program termination menu, as given below in Fig. 12.

```
-----  
  
----- O R T E P   T E R M I N A T I O N   O P T I O N   M E N U -----  
  
  
  
  
CONFIRM END OF ORTEP RUN *FINISH*      (23)  
OR RECALL ORTEP FOR A NEXT PLOT      (24)  
PREPARE OUTPUT FILE FOR HARDCOPY     (25)  
IDENTIFY ATOM BY CORRELATION         (26)  
UPDATE INST LOOKASIDE BUFFER OR INPUT (27)  
MODIFY CRYSTAL STRUCTURE DATA       (28)  
  
ENTER/VERIFY SELECTION NUMBER ==> _  
  
-----
```

Fig. 12. Program Termination Menu

From this the user may choose any of these actions as described in more detail in the following.

4.7.1 Terminate the ORTEP-G Program

To finish the ORTEP-G-program, END (option 23) must be confirmed on this menu. The program then terminates immediately and the CLIST will receive control.

4.7.2 Call for a Next Illustration

If the user wishes to produce another illustration or to find a better view of the plot, the EXEC panel **must** be recalled first.

4.7.3 Prepare Files for Hardcopy Plot

The data and options which together define a given illustration are stored automatically into two sequential data sets consisting of 80-character logical records in the ORTEP card format. The first one contains the crystal structure data, if given, and is defined by the FORTRAN file definition statement FT32F001. The second file holds the EXEC card and changed or inserted instructions, if any. This data set is allocated to the FORTRAN file definition statement FT33F001. These files are used later to generate job files for a batch execution. The file tailoring output will be directed to a sequential file provided by the command procedure, as described in section 5, where such a tailored output could be submitted to the background. After completion the program waits for a next choice.

4.7.4 Identify an Atom by Correlation

If no atom labels have been drawn (for clarity of the illustration), the user may identify single atoms on the display after selection of the related command. After positioning of the crosshair cursor, any gray key of the keyboard must be pressed. The name of the identified atom together with his ADC will be then displayed on the screen. Then

the user may select another atom, if desired. After pressing of the END (PF3) key the program termination menu receives control.

4.7.5 Update the Instruction Lookaside Buffer

As already outlined in chapter 4.2.3 a simple buffering technique has been implemented to repeat a sequence of added instructions automatically together with other instructions just inserted between the repetitions. However, it is often desirable, that the user may exercise control over the contents of the instruction lookaside buffer, for example, to reset the buffer to those instructions which are supplied from the input file FT05F001. To do this, the user must choose option 27 on this panel for calling the appropriate selection menu. If all operations have been completed, the program returns to the termination option menu after depressing of the PF3 key.

4.7.6 Modify the Crystal Structure Data

Once prepared, there is normally no need to change the crystallographic data. On the other hand, whenever this happens, entering a number of 28 causes a modification panel to be activated. Further informations on using this feature are given in chapter 4.3.6. Pressing of the PF3 key results in a redisplay of the termination menu.

4.8 Examples

This chapter contains a number of examples of figures produced with the ORTEP-G program on a mechanical plotter (VERSATEC).

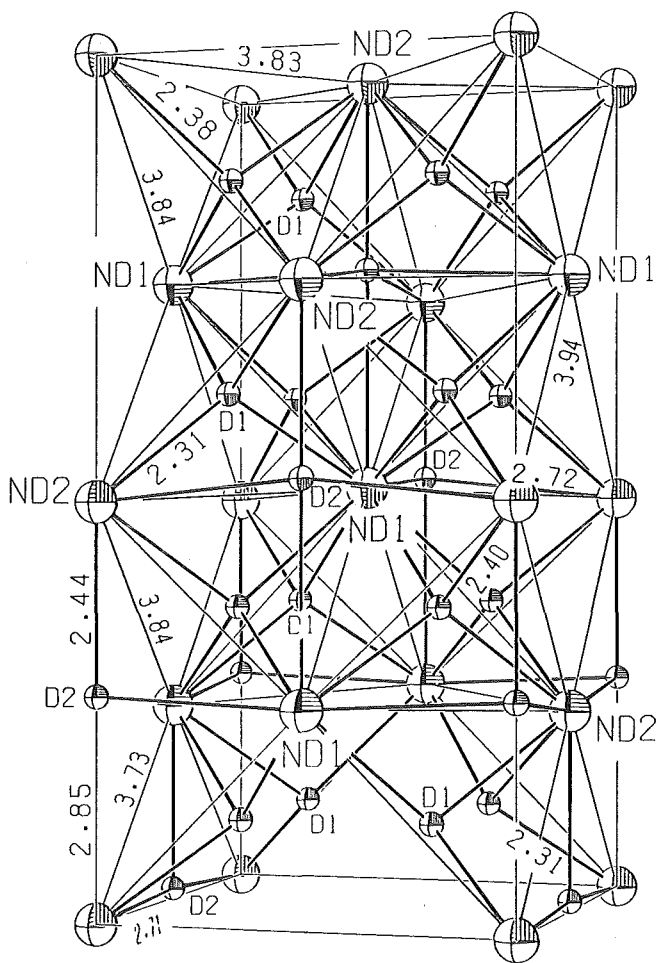


Fig. 13. Contents of the unit cell (in the a-c plane) for NdD(sub2.36)/7/. The instructions 901,913 and 915 have been used to place distance labels and atom labels.

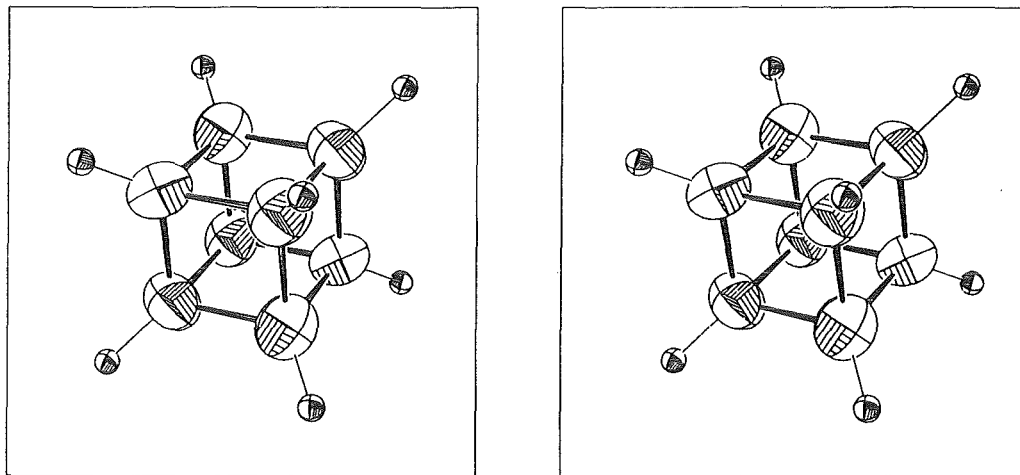


Fig. 14. Stereoscopic pair of perspective projections of Cubane/3/.

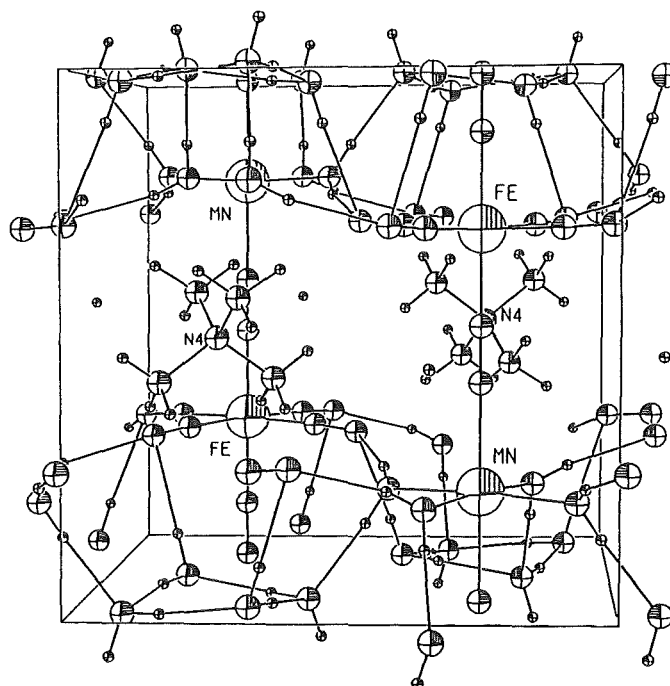


Fig. 15. Representation of a cyano-bridged chain structure with two formula units in the tetragonal cell. Some characteristic bonds are drawn to figure out the spatial configuration of $N(CH_3)_4 Mn Fe (CN)_6 \cdot 8 H_2O$.

5. Executing ORTEP-G on OS/VS2 MVS-TSO

5.1 Standard Input File

With respect to an "old" ORTEP user the whole well known card input may be supplied to the ORTEP-G program with minor changes only. In this version, the compound identification has been omitted from input. The EXEC card has been rewritten now to hold the minimum bond length. According to the input mode on the EXEC panel or card the user must predefine standard input data on cards or a similar source as given, for example, below:

IFILE=-1 (from sequential file)

```
ORTEP                2
EXEC -1021036100000 30.052.000.030.0 22.022.0 0.0 0.0 0. -30. .90-.50
CELL      10.00   10.00   10.00   90.00   90.00   90.00
LATICE    A  F
SYMTRY    X,Y,Z
SYMTRY    X,-Y,-Z
SYMTRY    -X,Y,-Z
SYMTRY    -X,-Y,Z
ATOM      MG1    0.0    0.0    0.0    0.005
ATOM      MG2    0.75   0.75   0.75   0.010
ATOM      MG3    0.25   0.25   0.25   .00001
ATOM      CU     0.37000 0.37000 0.37000 0.015
SEQ       PRECEDE 1
VSC       1     2 3 2 3 1 4 4.90 5.100.0001 0.0 0.0 0.0 0.
SEQ       PRECEDE 1
VSC       2     4 4 4 4 3 2 3.20 3.550.0300 0.0 0.0 0.0 0.
SEQ       PRECEDE 1
VSC       3     5 5 5 5 1 3 9.99 10.010.0001 0.0 0.0 0.0 0.
SEQ       PRECEDE 11
INST      204     4.     2.     0.     1.     0.     1.
END
FINISH
```

IFILE=0 (from BDF)

```
ORTEP                2
EXEC 0010136100000 30.052.000.030.0 11.011.0 0.0 0.0 0.0 0.0 .90-.50
END
FINISH
```

IFILE=1 (from CRT)

```
ORTEP          2
EXEC    1
END
FINISH
```

The parameter NPLOT on the ORTEP card (=2) indicates that the program will be used in an interactive environment. For a batch run this parameter must be set to 1.

5.2 Storage and Retrieval of ORTEP-G Data

Several FORTRAN files are used for permanent or temporary data gathering during an ORTEP-G run. Some of them are not necessary for running ORTEP-G in batch processing environment. Tabel 1 shows all used data files.

TABLE 1. Summary of ORTEP-G Data Files

DD-Name	Symbolic Name	Purpose
FT05F001	NTIN	Input file
FT06F001	NTOUT	Output file
SF20	NTAPEE	Scratch file for saved sequences in mode 1
SF23	NTAPEA	Crystallographic Binary Data File (BDF)
FT32F001	-	Scratch file for crystal structure data
FT33F001	-	Scratch file to hold EXEC/SEQ/INST cards
FT34F001	-	Scratch file (instruction lookaside buffer)
FT35F001	-	Scratch file
FT36F001	-	Scratch file for hardcopy ouput

5.3 CLIST

With respect to an efficient application of the computer code a command procedure has been developed which performs all necessary data set allocations due to user requirements, calls the ORTEP-G-program and releases all data sets after program stop. Furthermore, the JCL-file may be completed and submitted to the background, if desired.

After LOGON the user may start the program by entering the following TSO command:

```
ex 'tso352.tx.clist(ortep)'
```

A list of the CLIST-procedure ORTEP is given in Appendix B. First, a title will be printed. Next, the user is prompted for the name of an existing data set containing all crystal structure data, if any. Other alternatives depending on the input mode are explained in chapter 5.1.

ATOM(XX) INPUT EXISTS ON DATA SET (NO, RETURN) :

On the other hand, the user is required to enter a name for a new data set being allocated. After completion the next action of the user is to enter the name of a XRAY binary data file, if it exists.

ENTER DATA SET NAME OF (XRAY) BDF (NO,RETURN) :

If the user wishes to hold the crystallographic input data or to hold the EXEC card and instruction cards, respectively, on a sequential file, he may enter a data set name upon request:

ENTER NEW DATA SET NAME TO HOLD ATOM(XX) INPUT :

ENTER NEW DATA SET NAME TO HOLD EXEC/INST INPUT :

If not, temporary files will be allocated by the CLIST. If all allocations have been done successfully, the primary option menu appears on the 3277 screen indicating that the program is ready for use. From this menu the user must select the EXEC operation for the first illustration to define the execution mode and some graphical preliminaries. After program stop the message TERMINATE appears on the alphanumeric screen. Then the user has to decide whether a hardcopy plot should be prepared (assumed that he had selected option 25 on the termination option menu (see 4.7.3)), or not.

PLOT NO()/ON NOVA PRINTER(1)/VERSATEC(2)/XYNETICS(3) :

The printout of the last run may be routed to a local printer after

answering the next question. Last the message FINISH OF ORTEP is printed and the TSO receives control.

Acknowledgement

The author is indebted to Dr. H. Guth for many helpful discussions on crystal structure analysis and on using the ORTEP-2 program.

References

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- /4/ Stewart,J.M. et al., The XRAY system of crystallographic programs, Technical Report TR-446, Computer Science Center, University of Maryland, March 1976
- /5/ IBM 3277 Graphics Attachment Support (Programming RPQ P09013) Program Reference and Operations Manual Program Number 5799-AXX
- /6/ Yvon,K. et al., J. Appl. Cryst., 10(1977), p.73-75
- /7/ Knappe,P. et al., J. of the Less-Common Metals, 95(1983), p.323-333

Appendix A: Card Formats for ORTEP-G Program

Each record consists of a record type field of six characters, followed by a data field of variable length. Some of them may differ from the original ORTEP-2 cards in order to hold more input information.

ORTEP - program calling card.

Format(A2,A4,1X,A2,A4,I7)

cols specified punching or function of the field.
1-5 ORTEP
6 blank
20 (1)/(2) plot output (on plotter file)/(on CRT)

EXEC initialize new plot

Format(A2,A4,1X,I2,12I1,I2,3F4.2,5F4.1,2F4.0,2F4.1,F4.2,F4.1)

cols specified punching or function of the field.
1-4 EXEC
5-6 blank
7-8 INPUT (blank)/(1)(-1) enter data from (NFILEA)/(CRT)/(cards)
9 EXECMODE (blank)/(1) (do)/(do not) generate instr. sequence
10 PLOTTYPE (blank)/(1)/(2)/(3) plot (input)/(molecule)/(cell)/(atom coordinates)
11 OVERLAP (blank)/(1) (do not)/(do) correct for overlap
12 STEREO (blank)/(1)/(2) (single view)/(stereo in red and blue)/(stereo in red and green)
13 PLOTAXES (1/2/3/4/5/6) x-y axes (ab/ba/ca/ac/bc/cb)(blank=1)
14 ELIPSOID (1/2/3/4/5/6) ellipsoid type (point only)/(spheroid)/(envelope)/(princ. ellip.+envelope)/(princ. ellip.+env.+axes)/(ellip. with octant shading) (blank=3)
15 H-ATOMS (1/2/3/4) hydrogen atoms (excluded)/(included and sorted to bottom of atom list)/(included as spheres r=0.1Å and sorted)/(not sorted or treated differently to non-H-atoms) (see note)
blank=1 if execmode=0 and blank=4 if execmode=1
16 SYMBOLS (blank)/(1) (do not)/(do) draw atom symbols
17 CALC BLA (blank)/(1) (do not)/(do) calc bond angles/UIJ d.c.s
18 DRAW BL (blank)/(1) (do not)/(do) draw bond lengths on plot
19 AUTOSCAL (blank)/(1) (do not)/(do) suppress automatic scaling
20 PRINT (blank)/(1) (do not)/(do) limit atom/bond search o/p
21-22 BONDTYPE (-n)/(+n) bond line type (blank=1) see note below. magnitudes 0,1,2,3,4,5 form bonds with 0,2,3,5,9,17 lines resp. (-n) bonds terminate only at ellipsoids, (+n) bonds terminate at ellipsoids *or* at tangent cone with apex at the viewpoint
23-26 minimum bond length (blank=0.05Å) see note below.
27-30 maximum bond length (blank=2.0Å) see note below.
31-34 radius of stick bond (blank=0.03Å) see note below.
35-38 ellipsoid probability scale (blank=1.54 *or* =.1Å if col.14=2)
39-42 x-dimension of plot in inches (blank=11.0 in.)
43-46 y-dimension of plot in inches (blank=11.0 in.)
47-50 view distance in inches (blank=automatic, negative=infinity)

51-54 plot margin in inches (blank=0.1*x-dimension in.)
+or+ if col.10=3 atom input no. for coordination search.
55-58 ROTATION about x-axis of origin in degrees (blank=0.0)
59-62 ROTATION about y-axis of origin in degrees (blank=0.0)
63-66 x-displacement of atom symbols in inches (blank=0.0 in.)
67-70 y-displacement of atom symbols in inches (blank=-.5 in.)
71-74 height of atom symbols in inches (blank=automatic)
75-78 plot scale used if col.19=1 in inches/Å (blank=1.in./Å)

Note... Bond type, max. bond length and stick radius parameters refer +only+ to the non-hydrogen atoms if col.15 is 2 or 3. In this case the equivalent hydrogen parameters are preset at the values 1, 1.2Å (min=.5Å), 0.001Å (for line bond), resp.

CELL cell constant card.
Format(A2,A4,7X,3F8.3,3F9.5)

cols specified punching or function of the field
1-4 CELL
5-13 blank
14-21 a cell dimension or a* reciprocal cell dimension
22-29 b cell dimension or b* reciprocal cell dimension
30-37 c cell dimension or c* reciprocal cell dimension
38-46 cos alpha or alpha (degrees) or cos alpha* or alpha* (degrees)
47-55 cos beta or beta (degrees) or cos beta* or beta* (degrees)
56-64 cos gamma or gamma (degrees) or cos gamma* or gamma* (degrees)

Note... Quantities must be either all in direct space or all in reciprocal space. Angles must a&l&l be given as either cosines or in degrees.

LATICE centricity identification card.
Format(A2,A4,2X,A1,2X,A1)

cols specified punching or function of the field
1-6 LATICE
9 C=centric cell, A=acentric cell
12 designation of lattice type P,I,R,F,A,B,C one of the foregoing must be punched

SYMTRY symmetry operation card (maximum of 96)
Format(A2,A4,66A1)

cols specified punching or function of the field
1-6 SYMTRY
7-72 general equivalent position. The symmetry of the space group is indicated by supplying the set of general equivalent positions. Each equivalent position is specified on a separate SYMTRY card. A simple rule is that any general equivalent position in the international tables may be written verbatim with the following conventions,

(1) minus signs precede the negative quantity,
e.g. -x for x-bar.

- (2) fractions are written with the slash,
e.g. 1/2 for one-half.
- (3) blanks are ignored.

Note.. 1/2-x or -x+1/2 are both acceptable formats.

Note.. Do not punch any operations through the center if space group is coded centric on =LATICE= card.

SPCGRP space group symbols (may replace LATICE and SYMTRY cards)
Format(A2,A4,1X,35A1)

cols specified punching or function of the field

1-6 SPCGRP

8-72 Hermann Mauguin symbol for the space group (see App. E).
Adjust to the left of the field. Symmetry operations are separated by a slash or by a blank.

(1) Minus signs precede the negative quantity,
e.g. -x for x-bar.

(2) Screw axes are given by two integers that are not separated by a blank, e.g. P 21/C

Note.. For centrosymmetric groups, the programme assumes the setting having the centre at the origin.
For R-space groups the hexagonal setting is assumed.
R-space groups with rhombohedral axes must be simulated using LATICE- and SYMTRY cards corresponding to a triclinic description.

SYMHEL helicoidal symmetry operation card
Format(A2,A4,1X,F14.3,9X,F15.3,9X,F15.3,3I3)

cols specified punching or function of the field

1-6 SYMHEL

8-21 tx (x coordinate of the axis)

31-45 ty (y coordinate of the axis)

55-69 tz (phase displacement along the axis)

70-72 l parameter

73-75 m parameter

76-78 n parameter

Transformed helicoidal coordinates x_1 are obtained from input coordinates x by the transformation $x_1 = t + sx$ where $t = (t_1, t_2, t_3 + l/m)$ and $s = a$ counterclockwise rotation of $l \cdot m/n$ cycles about c^* axis. For example, the pauling and corey right-handed alpha helix repeats after 5 turns and 18 residues and can be represented by 18 symmetry cards with $n=18, m=5, l=0, 1, 2, \dots, 17, t_1=t_2=t_3=0$.

The input atom list contains the content of one residue.

ATOM atom parameters card (maximum of 100)
Format(A2,A4,1X,A4,A2,3F8.4,F6.4,5X,I1)

cols specified punching or function of the field

1-4 ATOM
5-6 blank
8-13 atom identification
14-21 x coordinate
22-29 y coordinate
30-37 z coordinate
38-43 isotropic temperature factor if supplied in this card --
treated as B above 0.3 and as U below 0.3, $B = 78.96*U$.
49 coordinate system designator
(blank) fractional crystal (dimensionless)
(1) absolute crystal (in Å and along unit cell vectors)
(2) cartesian (in Å)

ATOMC atomic parameters in cylindrical coordinates (maximum of 100)
Format(A2,A4,1X,A4,A2,3F8.4,F6.4,6X,2F8.4)

cols specified punching or function of the field
1-5 ATOMC
6 blank
8-13 atom identification
14-21 r in Å (cylindrical coordinate)
22-29 phi in degrees (cylindrical coordinate)
30-37 z in Å (cylindrical coordinate)
38-43 isotropic temperature factor if supplied in this card --
treated as B above 0.3 and as U below 0.3, $B = 78.96*U$.
50-57 xzero in Å
58-63 yzero in Å

Note... In order to understand the cylindrical representation
we refer to the cartesian representation. In both
systems the z parameter is identical and the origin of
the cylindrical system may be placed anywhere in the
cartesian plane x-y.

B, U, BIJ, UIJ, and BETA temperature factor cards
Format(A2,A4,1X,A4,A2,6F8.4)

cols specified punching or function of the field
1-4 appropriate label B, U, BIJ, UIJ or BETA
5-6 blank
8-13 atom identification (see 3.6)
14-21 b or u or b11 or u11 or betall (see 3.6)
22-29 b22 or equivalent
30-37 b33 or equivalent
38-45 b12 or equivalent
46-53 b13 or equivalent
54-61 b23 or equivalent

RADIUS replace temperature factor by a sphere of a given radius.
Format(A2,A4,1X,A4,A2,F8.3)

cols specified punching or function of the field
1-6 RADIUS
8-13 atom identification
14-21 radius (Å) of the sphere representing the atom on the

drawing*

*Note ... radius is scaled by both SCAL1 and SCAL2 of the 600 instructions.

ATOMD atom deletion card
Format(A2,A4,1X,A4,A2)

cols specified punching or function of the field
1-6 ATOMD
8-13 atom identification

Note... When an atom is deleted the temperature factors for that atom are lost.

RENAME card to change atom identification
Format(A2,A4,1X,A4,A2,1X,A4,A2)

cols specified punching or function of the field
1-6 RENAME
8-13 old atom identification
15-20 new atom identification

REPOSN card to reposition atom in atoms list
Format(A2,A4,1X,A4,A2,I4)

cols specified punching or function of the field
1-6 REPOSN
8-13 atom identification
14-17 new position number in the atom list.

SEQ card to modify generated instruction sequence
(!must! precede each =INST= or =VSC= card in automatic execution mode)
Format(A2,A4,4X,A4,3X,I3)

cols specified punching or function of the field
1-6 SEQ
11-17 alpha text = 'REPLACE' or 'PRECEDE' when followed by INST card
or = 'PRECEDE' when followed by VSC card*
18-20 sequence number of automatically generated instruction used to control the entry of the following =INST= or =VSC= card *

*Note ... VSC's are stored in a separate array and cannot replace an instruction. The =SEQ= card simply enables the inclusion of a VSC in this array to be sequenced prior to the execution of a given instruction. This is in contrast to when a =INST= card follows a =SEQ= card containing 'PRECEDE' as this causes the instruction to be physically inserted into the instruction sequence.

Any change to the automatic options on the EXEC card will alter the instruction sequence numbering and may therefore invalidate these modifications.

VSC vector search code
(applies to 101,102,402/412,405/415,406/416,407 search,
or 801/811,802/812,803/813 bond plotting instr.)
Format(A2,A4,I4,2X,5I3,I3,2F6.2,F6.4,5F6.2)

cols specified punching or function of the field

1-3 VSC
4-6 blank
7-10 serial number in the VSC-array (array max. is 10)
11-12 blank
13-15 ANC 1)
)origin ANR)
16-18 ANC 2)
19-21 ANC 3) irrelevant for 801,811 instructions
)target ANR)
22-24 ANC 4)
25-27 bondtype (-n)/(+n) bond line type (see note 1)
magnitudes 0,1,2,3,4,5 form (no bond)/(stick bond, edges only)/
(lines drawn at 90)/(at 45)/(at 22.5)/(at 11.25 degrees apart)*
(-n) bonds terminate only at ellipsoids, (+n) bonds terminate
at ellipsoids *or* at tangent cone with apex at the viewpoint
28-30 pen color for bonds (black(0), red(2), blue(3), green(4))
(for the XYNETICS plotter only)
31-36 DMIN (Å) (see note 1)
37-42 DMAX (Å) (see note 1)
43-48 bond radius (Å) (see note 1)
49-54 perspective bond label height (inches) omit if blank)
55-60 perpendicular displacement (inches)) see
61-66 nonperspective label height (inches)) notes
67-72 perpendicular displacement (inches)) below
73-78 (-1)/(0)/(1) for (1)/(2)/(3) decimal places)

Note 1 ...Bond type, bond radius, and bond label parameters
apply only to 802/812 and 803/813 instr. Origin ADR
target ANR, DMIN and DMAX are ignored by 801/811
instructions. If cols. 49-54 are blank the bond
labels (i.e. length values) are *not* drawn.

Note 2 ... (polyhedra bond plotting facility for 802,803,)
(812,813 instructions is indicated by a negative)
(sign in cols. 49-54.)
(cols specified punching or function of field)
(49-54 -ANC 1)
() polyhedra ANR)
(55-60 ANC 2)
(61-66 polyhedra DMIN (Å))
(67-72 polyhedra DMIN (Å))

SYMBOL alphanumeric information that can be output on the plotter by
the instructions number 902, 903, and 913 (see 4.4).
Format(A2,A4,18A4)

cols specified punching or function of the field
1-6 SYMBOL

7-78 alphanumeric information centered about columns 42 and 43

SVSTAR card to indicate the beginning of a sequence to be saved
(manual mode only)
Format(A2,A4)

cols specified punching or function of the field
(manual mode only)

1-6 SVSTAR

SVEND card to indicate the end of a saved sequence
(manual mode only)
Format(A2,A4)

cols specified punching or function of the field

1-5 SVEND

SVEEXEC card for the execution of the saved sequence of instructions
(manual mode only)
Format(A2,A4)

cols specified punching or function of the field

1-6 SVEEXEC

INST structure analysis (101,102,105,106 instructions)
Format(A2,A4,2X,I1,3X,I3,5F9.2)

cols specified punching or function of the field

1-6 INST

13-15 (101)/(102)/(105)/(106) for (distances)/(distances and angles)/
(spheres of enclosure)/(reiterative spheres of enclosure)

16-24 ADC 1
)origin ADR

25-33 ADC 2

34-42 ANC 1
)target ANR

43-51 ANC 2

52-60 DMAX(Å)

Note... These instructions are screened by the VSC array.

INST thermal eigenvectors (103 instruction)
Format(A2,A4,6X,I3)

cols specified punching or function of the field

1-6 INST

13-15 103 for amplitudes and direction cosines of thermal ellipsoids

INST plotter and CRT control (201,202,211 instructions)
Format(A2,A4,6X,I3,2F9.0)

cols specified punching or function of the field

1-6 INST

13-15 (201)/(202)/(211) (initialize plotter)/(advance plotter)/

(start CRT)
16-24 plotter movement in x direction (inches) only if 202
25-33 plotter movement in y direction (inches) only if 202

INST pen colour for bonds (203 instruction)
Format (A2,A4,6X,I3,F9.0)

cols specified punching or function of the field
1-6 INST
13-15 203 for change pen
16-24 (0 or 1, black)/(2, red)/(3, blue)/(4, green)

Note... This instruction is screened by the VSC card

INST pen colour for atoms (204 instruction)
(for the XYNETICS plotter only)
Format (A2,A4,6X,I3,3F9.0)

cols specified punching or function of the field
1-6 INST
13-15 204 for change pen of up to three atoms
16-24 ANC 1 (blank, if not changed)
25-33 (2, red)/(3, blue)/(4, green)
33-42 ANC 2 (blank, if not changed)
43-51 (2, red)/(3, blue)/(4, green)
52-60 ANC 3 (blank, if not changed)
61-69 (2, red)/(3, blue)/(4, green)

INST plot boundary (301,302,303 instructions)
Format(A2,A4,6X,I3,4F9.2)

cols specified punching or function of the field
1-6 INST
13-15 (301)/(302)/(303) for (defining plot dimensions)/
(title rotation)/(retrace displacement)
16-24 plot limit in x direction (inches) *or* title rotation angle
(degrees) *or* displacement parameter (inches) depending on
code in cols 13-15.
25-33 plot limit in y direction (inches))
34-42 view distance (inches))only for 301 in cols 13-15
43-51 border (inches))

INST explicit update of atoms array (401/411 instructions)
Format(A2,A4,2X,I1,3X,I3,7F9.0)

cols specified punching or function of the field
1-6 INST
9 (blank)/(1) for (do not)/(do) continue on following card
13-15 (401)/(411) for (add)/(eliminate) specified atoms from atoms
array.
16-24 ADC 1)
)ADR 1)
25-33 -ADC 2)
34-42 ADC 3) Note.. Individual atoms may be entered as
)ADR 2) single ADC's. An ADR is recognized by a

43-51 -ADC 4) positive ADC followed by a negative ADC.
52-60 ADC 5)
)ADR 3)
61-69 -ADC 6)
70-78 ADC 7 (the ADC's and ADR's may continue on following card
 if col.9=1)

INST update atoms array
 (402/412,403/413,404/414,405/415,406/416,407 instructions)
 Format(A2,A4,6X,I3,7F9.2)

cols specified punching or function of the field
1-6 INST
13-15 (402)/(403)/(404)/(405)/(406)/(412)/(413)/(414)/(415)/(416)/
 (407) for
 sphere add)/(box of enclosure add)/(triclinic box add)/
 (convolute add)/ (reiterate convolute add)/(sphere subtract)/
 (box subtract)/(triclinic box subtract)/
 (convolute subtract)/(reiterate convolute subtract)/
 (same as 406 except sites related by pure cell translation
 are ignored)

16-24 ADC 1
)origin ADR

25-33 ADC 2

34-42 ANC 1

)target ANR

43-51 ANC 2

52-60 dmax (Å) for 402/412,405/415,406/416 instructions *or*

 a/2 (Å))

61-69 b/2 (Å)) for 403/413,404/414 instructions

70-78 c/2 (Å))

Note...402/412, 405/415, 406/416 instructions are screened by
 VSC array

INST clear atoms array (410 instruction)
 Format(A2,A4,6X,I3)

cols specified punching or function of the field

1-6 INST

13-15 410 to zero atoms array

INST plot orientation (501 instruction)
 Format(A2,A4,6X,I3,5F9.0,18X,I1)

cols specified punching or function of the field

1-6 INST

13-15 501 definition of reference cartesian system

16-24 ADC 1 origin

25-33 ADC 2

)vector v1

34-42 ADC 3

43-51 ADC 4

)vector v2

52-60 ADC 5

78 (blank)/(1) for (type a)/(type b) description

INST plot orientation (502,503 instructions)
Format(A2,A4,2X,I1,3X,I3,7F9.2)

cols specified punching or function of the field
1-6 INST
9 (blank)/(1) for (do not)/(do) continue instruction on next card
13-15 (502)/(503) for (rotate ref. system)/(rotate working system)
16-24 (1)/(2)/(3)/(-1)/(-2) for rotate about (x)/(y)/(z)/(120 deg.
about body-diagonal)/(240 deg. about body-diagonal)
25-33 rotation angle (degrees) positive is counter-clockwise looking
down the axis towards the origin
34-42 as for 16-24)
43-51 as for 25-33)
52-60 as for 16-24)only if 502 in cols 13-15
61-69 as for 25-33)
70-78 as for 16-24)

INST plot orientation (504 instruction)
Format(A2,A4,6X,I3,3F9.2)

cols specified punching or function of the field
1-6 INST
13-15 (504) to translate the origin
16-24 translation of origin along x-ref.(inches)
25-33 translation of origin along y-ref.(inches)
34-42 translation of origin along z-ref.(inches)

Note ... This instruction should not be used, if the
ellipsoids have internal structure; the octants
may not be the same for the two projections.
For additional drawings the origin must be first
reset to its initial value by a supplemental 504
instruction/3/.

INST overlap correction (511 instruction)
Format(A2,A4,6X,I3,F9.3)

cols specified punching or function of the field
1-6 INST
13-15 511 to correct plot for overlap
16-24 overlap margin (inches)

INST position and scaling
(601,602,603,604,611,612,613 instructions)
Format(A2,A4,6X,I3,4F9.2)

cols specified punching or function of the field
1-6 INST
13-15 (601)/(602)/(603)/(604)/(611)/(612)/(613) for (explicit)/(scale
only)/(center only)/(center and scale)/(increment position and
increment scale)/(increment position and scale)/(increment
scale and center)
16-24 x position of origin (inches) if 601 or 602 in cols 13-15

x increment (inches) if 611 or 612 in cols 13-15
25-33 y position of origin (inches) if 601 or 602 in cols 13-15
y increment (inches) if 611 or 612 in cols 13-15
34-42 scale for plot if 601 or 603 in cols 13-15
scale increment if 611 or 613 in cols 13-15
43-51 ellipsoid scale (blank = 1.54 for 50 percent probability)

INST atom plotting
(701,702,703,704,711,712,713,714 instructions)
Format(A2,A4,2X,I1,3X,I3,36X,3F9.2)

cols specified punching or function of the field
1-6 INST
9 (blank)/(1) for (no)/(further) parameters on the following card
13-15 (701)/(702)/(703)/(704)/(711)/(712)/(713)/(714) for (shaded
football)/(football)/(open model)/(boundary only)/(as 701 less
output)/(as 702 less output)/(as 703 less output)/
(as 704 less output)
52-60 symbol height (inches))
61-69 parallel offset (inches)) for symbols
70-78 perpendicular offset (inches))

INST compound ellipsoid (705/715 instructions)
Format(A2,A4,2X,I1,3X,I3,4F9.0,3F9.2)

cols specified punching or function of the field
1-6 INST
9 (blank)/(1) for (no)/(further) parameters on the following card
13-15 (705)/(715) for (other types of ellips.)/(as 705 less output)
16-24 (0)/(1)/(3)/(4) for (no ellipsoid components)/(boundary ellipse
only)/(principal ellipses only)/(boundary and principal
ellipses)
25-33 (-1)/(0)/(3)/(4)/(5)/(6) for back side of principal ellipses
with (solid line)/(omitted)/(4 dots)/(8 dots)/(16 dots)/
(32 dots)
34-42 (0)/(1)/(positive integer, n) for forward principal axes
(omitted)/(plotted)/(plotted and shaded with n-1 lines)
43-51 (0)/(positive integer, n) for reverse principal axes
(plotted with n dashes))
52-60 symbol height (inches)) for symbols
61-69 parallel offset (inches))
70-78 perpendicular offset (inches))

INST 700 series continue for boundary retracing and plot constraints
Format(A2,A4,11X,4F9.2)

cols specified punching or function of the field
1-6 INST
13-15 instruction code (701 - 715) of preceding card
16-24 a0, increase in radial dimension (inch) for boundary retracing
25-33 a1, rate of increase in radial dimension with height for
retracing.
34-42 ANC 1
)ANR specifying sites in atoms list to be plotted
43-51 ANC 2

INST explicit stick bonds (801/811 instructions)
Format(A2,A4,2X,I1,3X,I3,3F9.0,F9.4,F9.0,F9.2,F9.0)

cols specified punching or function of the field
1-6 INST
9 (blank)/(1) for (no)/(yes) continue on following card
-identical format-
13-15 (801)/(811) plot explicit stick bonds (with)/(less) full
listing
16-24 ADC 1
)bond
25-33 ADC 2
34-42 bond type
43-51 bond radius (Å)
52-60 height of the symbol (inches)
61-69 pen color for bond

Note ... The label offset parameters are specified by the
first (serial no. 1) VSC in the VSC array

INST bond plotting (802/812, 803/813, instructions)
Format(A2,A4,2X,I1)

cols specified punching or function of the field
1-6 INST
13-15 (802)/(803)/(812)/(813) for (implicit stick bonds)/(implicit
line bonds)/(802 less printout)/(803 less printout)

Note... Bond parameters specified by VSC array

INST labels (901,902,903,904,905,906,908,909,913,914,915,916
instructions)
Format(A2,A4,2X,I1,3X,I3,2F9.0,5F9.3)

cols specified punching or function of the field
1-6 INST
9 (blank)/(1) for (no)/(yes) symbol no. on following card
- for 908 or 909 -
13-15 (901)/(902)/(903)/(904)/(905)/(906)/(908)/(909)/(913)/(914)/
(915)/(916)
for (chemical symbol)/(regular title)/(projected vector title)/
(projected bond label, 1 decimal places)/(2 decimal places)/
(3 decimal places)/(centered symbol, pen up)/(centered symbol,
pen down)/(perspective vector title)/(perspective bond label,
1 decimal places)/(2 decimal places)/(3 decimal places)
16-24 ADC 1 blank for 902
) label ADR
25-33 ADC 2 blank for 901 or 902
34-42 x edge reset (inches)
43-51 y edge reset (inches)
52-60 lettering height (inches)
61-69 parallel offset (inches)
70-78 perpendicular offset (inches)

Note... Alphanumeric information obtained from preceding SYMBOL card

INST 908,909 continue for centered symbol number
Format(A2,A4,9X,F9.0)

cols specified punching or function of the field

1-6 INST

13-15 instruction code (908 or 909) of preceding card

16-24 centered symbol number (0-14) symbols range from a square to a five-pointed star (no. 14)

END terminate current plot or plot tape
Format(A2,A4)

cols specified punching or function of the field

1-6 END

Appendix B: CLIST Procedure for ORTEP-G

```
PROC 0
CONTROL END(ENDO) NOFLUSH NOMSG
GLOBAL &USER
GLOBAL &NAME &ACCT
ERROR DO
    WRITE ERROR EXIT: cc=&lastcc cmd=&syspcmd
    RETURN
    ENDO
ATTN DO
WRITE DATA SETS MUST BE FREED
GOTO ENDE
ENDO
EX 'TSOSYS.COMDPROC.CLIST(MSSCLEAR)'
WRITE *****
WRITE *           O R T E P   -   G           *
WRITE * (THERMAL ELLIPSOID PLOTTING PROGRAM) *
WRITE *****
WRITE
FREE F(FT05F001)
FREE F(FT06F001)
FREE F(GAAPLIB)
CONTROL MSG
ALLOC DA('TSOSYS.GAS.FONT') F(GAAPLIB) SHR
ATTRIB DCB1 LRECL(80) BLKSIZE(3120) RECFM(F B)
CONTROL NOMSG
SET &BDF=
SET &INST=
SET &ATOM=
WRITENR ORTEP-G INPUT EXISTS ON DATA SET (NO, RETURN) :
READ &ALL
IF &ALL= THEN +
DO
REREAD: +
WRITENR ENTER NEW DATA SET NAME TO HOLD ORTEP-G INPUT :
READ &ALL
IF &ALL= THEN GOTO REREAD
CONTROL MSG
ALLOC SPACE(1,2) TRACKS NEW USING(DCB1) DA(&ALL.)
COPY 'TSO352.DUMMY.DATA' &ALL. NONUM
CONTROL NOMSG
EDIT &ALL. DATA OLD NONUM
TOP
DEL * 500
IN ORTEP           2
IN EXEC   1
IN END
IN FINISH
S
END
FREE DA(&ALL.)
ENDO
ELSE +
```

```
DO
ALLOC F(INDATA) DA(&ALL.) SHR
OPENFILE INDATA
GETFILE INDATA
GETFILE INDATA
SET &IFILE=&SUBSTR( 8: 8,&INDATA)
IF &IFILE=0 THEN +
DO
WRITENR ENTER DATA SET NAME OF (XRAY) BDF (NO, RETURN) :
READ &BDF
IF &BDF ^= THEN +
ALLOC F(SF23) DA('&BDF') SHR
ENDO
CLOSFILE INDATA
FREE F(INDATA)
ENDO
/******/
WRITENR ENTER NEW DATA SET NAME TO HOLD ATOM(XX) INPUT :
READ &ATOM
IF &ATOM ^= THEN +
DO
ALLOC F(FT32F001) SPACE(1,2) TRACKS NEW USING(DCB1) DA(&ATOM)
ENDO
ELSE +
DO
ALLOC F(FT32F001) SPACE(1,2) TRACKS NEW USING(DCB1)
ENDO
WRITENR ENTER NEW DATA SET NAME TO HOLD EXEC/INST INPUT :
READ &INST
IF &INST ^= THEN +
DO
ALLOC F(FT33F001) SPACE(1,2) TRACKS NEW USING(DCB1) DA(&INST)
ENDO
ELSE +
DO
ALLOC F(FT33F001) SPACE(1,2) TRACKS NEW USING(DCB1)
ENDO
/**** ALLOCATE SCRATCH FILES ****/
ALLOC F(FT34F001) SPACE(1,2) TRACKS NEW USING(DCB1)
ALLOC F(FT35F001) SPACE(1,2) TRACKS NEW USING(DCB1)
ALLOC F(FT36F001) SPACE(1,2) TRACKS NEW USING(DCB1) DA(XRTHC.DATA)
FREE ATTRLIST(DCB1)
ATTRIB DCB3 LRECL(2240) BLKSIZE(2240) RECFM(F)
ALLOC F(SF20) SPACE(1) TRACKS USING(DCB3)
ALLOC F(SF22) SPACE(1) TRACKS USING(DCB3)
FREE ATTRLIST(DCB3)
ATTRIB DCB2 LRECL(133) BLKSIZE(3857) RECFM(F B A)
ALLOC DA(XRTPR.DATA) USING(DCB2) SPACE(5,2) TRACKS NEW
FREE ATTRLIST(DCB2)
ALLOC F(FT06F001) DA(XRTPR.DATA) SHR
COPY &ALL. XRTIN.DATA NONUM
ALLOC F(FT05F001) DA(XRTIN.DATA) SHR
CALL 'TSO352.ORT01.LOAD(TEMPNAME)'
EX 'TSOSYS.CMDPROC.CLIST(MSSCLEAR)'
WRITE == TERMINATE ==
```

```
WRITE
SET &JCL=0
SET &PRI=0
CONTROL NOMSG
COPY XRTIN.DATA &ALL. NONUM
FREE F(FT05F001 FT06F001)
DEL XRTIN.DATA
ALLOC F(FT05F001) DA(*)
ALLOC F(FT06F001) DA(*)
FREE F(FT32F001 FT33F001 FT34F001 FT35F001)
FREE F(SF20 SF22)
IF &PL ^= THEN FREE F(INDATA)
IF &BDF ^= THEN FREE F(SF23)
WRITE HARD COPY PLOT AS PREPARED WITHIN ORTEP-G (25)
WRITENR NO()/ON NOVA PRINTER(1)/VERSATEC(2)/XYNETICS(3) :
READ &PL
IF &PL ^= THEN +
DO
SET &JCL=1
EX 'TSO352.TX.CLIST(RDACCT) '
CONTROL MSG
COPY 'TSO352.DUMMY.DATA' XRJCL.CNTL NONUM
EDIT XRJCL CNTL NONUM OLD
TOP
DEL * 500
IN //IAK&USER.PP JOB &ACCT. ,&NAME
IF &PL=1 THEN +
DO
IN //&STR(*)MAIN ORG=RM009,CARDS=90
ENDO
ELSE +
DO
IN //&STR(*)MAIN LINES=10,ORG=RM007
ENDO
IF &PL=1 THEN SET &PLTYPE=&STR(VERSATEC)
IF &PL=2 THEN SET &PLTYPE=&STR(VERSATEC)
IF &PL=3 THEN SET &PLTYPE=&STR(XYNETICS)
IN // EXEC FGLG,PLOT=&PLTYPE,PARM.L='OVLY,LIST',LIB=IAK,
C * / /; /A
C * / ; ; ; ; ; ; ; ; //
C * / ; / ; * /
C * / ; / /A
IN // USER='ADI186.V1$1.GAS.LOAD'
IN //L.SYSLIN DD DDNAME=SYSIN
IN // DD DSN=TSO352.ORTOV.DATA,DISP=SHR
IN //L.SYSLIN DD *
IN INCLUDE LOAD(ORTEPG)
IF &ATOM ^= THEN +
DO
in //G.FT32F001 DD DSN=&SYSPREF..&ATOM,DISP=SHR
ENDO
ELSE +
DO
IN //G.FT32F001 DD DSN=&STR(&&)INPUT,UNIT=SYSDA,SPACE=(TRK,(3,2)),
IN // DISP=(,DELETE),DCB=(LRECL=80,RECFM=FB,BLKSIZE=3120)
```

```

ENDO
IF &INST $\neq$  THEN +
DO
IN //G.FT33F001 DD DSN=&SYSPREF..&INST,DISP=SHR
ENDO
ELSE +
DO
IN //G.FT33F001 DD DSN=&STR(&&)INST1,UNIT=SYSDA,SPACE=(TRK,(3,2)),
IN // DISP=(,DELETE),DCB=(LRECL=80,RECFM=FB,BLKSIZE=3120)
ENDO
IN //G.FT34F001 DD DSN=&STR(&&)ILASB,UNIT=SYSDA,SPACE=(TRK,(3,2)),
IN // DISP=(,DELETE),DCB=(LRECL=80,RECFM=FB,BLKSIZE=3120)
IN //G.FT35F001 DD DSN=&STR(&&)INST2,UNIT=SYSDA,SPACE=(TRK,(3,2)),
IN // DISP=(,DELETE),DCB=(LRECL=80,RECFM=FB,BLKSIZE=3120)
IN //G.FT36F001 DD DSN=&STR(&&)INST3,UNIT=SYSDA,SPACE=(TRK,(3,2)),
IN // DISP=(,DELETE),DCB=(LRECL=80,RECFM=FB,BLKSIZE=3120)
IF &BDF $\neq$  THEN +
DO
IN //SF23 DD DISP=SHR,DSN=&BDF
ENDO
IN //SF20 DD UNIT=SYSDA,SPACE=(TRK,(3,2)),DISP=(NEW,DELETE),
IN // DSN=&STR(&&)SF20
IN //SF22 DD UNIT=SYSDA,SPACE=(TRK,(3,2)),DISP=(NEW,PASS),
IN // DSN=&STR(&&)SF22
IF &PL=3 THEN +
DO
IN //G.PLOTTAPE DD UNIT=T0800,VOL=SER=X352PP,LABEL=(,NL),DCB=DEN=2
ENDO
IF &PL=1 THEN +
DO
IN //G.PLOTPARM DD *
IN &STR(&&PLOT) XFACT=1.428 YFACT=1.214 &STR(&&END)
ENDO
IN //G.SYSIN DD *
OPENFILE FT36F001 INPUT
NEXT: +
GETFILE FT36F001
SET &INDATA=&FT36F001
IN &INDATA
IF &SUBSTR(1:6,&INDATA)=&STR(FINISH) THEN GOTO ENDIN
GOTO NEXT
ENDIN: +
CLOFILE FT36F001
IF &PL $\neq$ 3 THEN +
DO
IN // EXEC SVPLOT
IF &PL=1 THEN +
DO
IN //PLOT.SYSVECTR DD SYSOUT=B,DCB=(BLKSIZE=4000,LRECL=80,RECFM=FBA)
ENDO
ENDO
IN //
S
END
CONTROL MSG

```

```
WRITENR ENTER DATA SET NAME TO HOLD THE GENERATED JCL      :
READ &JCLSET
IF &JCLSET~= THEN +
DO
COPY XRJCL.CNTL &JCLSET NONUM
SUB &JCLSET
ENDO
ELSE +
DO
SUB XRJCL.CNTL
ENDO
ENDO
/*****/
WRITENR DO YOU WANT TO KEEP THE PRINTING OF THE LAST RUN ?
WRITENR NO() PRINT OUT VIA RJE(7/9) OR KEEP THE DATA SET(H) :
READ &OUT
IF &OUT= THEN GOTO ENDE
SET &PRI=1
IF &OUT=H THEN GOTO ENDE
SET &JCL=1
CONTROL NOMSG
EX 'TSO352.TX.CLIST(RDACCT)'
COPY 'TSO352.DUMMY.DATA' XRJCL.CNTL NONUM
EDIT XRJCL CNTL NONUM OLD
TOP
DEL * 500
IN //IAK&USER.PR JOB &ACCT.,&NAME
IN //&STR(*)MAIN ORG=RM00&OUT
IN //OUT EXEC PGM=IEBGENER
IN //SYSUT1 DD DSN=&SYSPREF..XRTPR.DATA,DISP=(OLD,DELETE)
IN //SYSUT2 DD SYSOUT=A
IN //SYSPRINT DD DUMMY
IN //SYSIN DD DUMMY
IN //
S
END
CONTROL MSG
SUB XRJCL.CNTL
WRITE PRINT OUT HOLD IN DATA SET XRTPR.DATA, WHICH WILL BE DELETED
WRITE AFTER COMPLETION OF THE SUBMITTED JOB
ENDE: +
CONTROL NOMSG
DEL XRTHC.DATA
FREE F(FT36F001)
IF &JCL~=0 THEN DEL XRJCL.CNTL
IF &PRI =0 THEN DEL XRTPR.DATA
        ELSE FREE DA(XRTPR.DATA)
WRITE ** FINISH ** END OF ORTEP-G ** FINISH **
END
```

Appendix C: Overlay Structure of ORTEP-G

ENTRY MAIN
OVERLAY ALPHA
INSERT PRELM, GENINS
INSERT DSGENI, DSVSC, DSINST, DSSEQ, DSSYMB
OVERLAY ALPHA
INSERT ORLEC
INSERT DSLATT, DSSYMT, DSATOM, DSATMC, DSATMD
INSERT DSCCELL, DSTEMP, DRSY, DSRNAM, DSRPOS
INSERT SPCGRP, BURZ, EQUI, BRA, DSSGRP
OVERLAY ALPHA
INSERT F200, F400, SEARC, F600
OVERLAY ALPHA
INSERT F500, F700, F1000
INSERT LAP500, LAP700
OVERLAY ALPHA
INSERT F800, BOND, LAP800
OVERLAY BETA(REGION)
INSERT SETCOR
INSERT XYDATA

Appendix D: JCL requirements for Batch Processing

```
//IAK352PP JOB (0352,143,POA2E),ABEL
//*MAIN LINES=10,ORG=RM007
// EXEC FGLG,PLOT=VERSATEC,PARM.L='OVLY,LIST',LIB=IAK,
// USER='ADI186.V1$1.GAS.LOAD',LIB=IAK
//L.SYSLIN DD DDNAME=SYSIN
// DD DSN=TSO352.ORTOV.DATA,DISP=SHR
//L.SYSIN DD *
  INCLUDE LOAD(ORTEPG)
//G.FT32F001 DD DSN=&&INPUT,UNIT=SYSDA,SPACE=(TRK,(3,2)),
// DISP=(NEW,DELETE),DCB=(RECFM=FB,LRECL=80,BLKSIZE=3120)
//G.FT33F001 DD DSN=&&INST1,UNIT=SYSDA,SPACE=(TRK,(3,2)),
// DISP=(NEW,DELETE),DCB=(RECFM=FB,LRECL=80,BLKSIZE=3120)
//G.FT34F001 DD DSN=&&ILASB,UNIT=SYSDA,SPACE=(TRK,(3,2)),
// DISP=(NEW,DELETE),DCB=(RECFM=FB,LRECL=80,BLKSIZE=3120)
//G.FT35F001 DD DSN=&&INST2,UNIT=SYSDA,SPACE=(TRK,(3,2)),
// DISP=(,DELETE),DCB=(LRECL=80,RECFM=FB,BLKSIZE=3120)
//G.FT36F001 DD DSN=&&INST3,UNIT=SYSDA,SPACE=(TRK,(3,2)),
// DISP=(,DELETE),DCB=(LRECL=80,RECFM=FB,BLKSIZE=3120)
//G.SYSIN DD *
ORTEP
EXEC -1021136100000 30.052.000.030.0 6.0 6.0 0.0 0.0 0.0-30. .90-.500.14 1.0
CELL 10.00 10.00 10.00 90.00 90.00 90.00
LATTICE A F
SYMTRY X,Y,Z
SYMTRY X,-Y,-Z
SYMTRY -X,Y,-Z
SYMTRY -X,-Y,Z
ATOM MG1 0.0 0.0 0.0 0.005
ATOM MG2 0.75 0.75 0.75 0.010
ATOM MG3 0.25 0.25 0.25 .00001
ATOM CU 0.37000 0.37000 0.37000 0.015
SEQ PRECEDE 1
VSC 1 2 3 2 3 1 4 4.90 5.10 .0010 0.0 0.0 0.0 0.0 0.0
SEQ PRECEDE 1
VSC 2 4 4 4 4 3 2 3.20 3.55 0.03 0.0 0.0 0.0 0.0 0.0
SEQ PRECEDE 1
VSC 3 5 5 5 5 1 3 9.99 10.01 .0010 0.0 0.0 0.0 0.0 0.0
END
FINISH
// EXEC SVPLOT
//
```

Appendix E: Space Group Symbols

The star preceding some of the symbols (do n o t include the star) indicates centrosymmetric space groups which have been described with several settings. The program generates only the setting with the centre of symmetry at the origin of the unit cell. The space group symbol must be entered left adjusted as given, i.e. blanks included.

W A R N I N G :

A symbol that does not figure in this list may yield wrong equipoints.

TRICLINIC

P 1 P -1

MONOCLINIC

P 2	P 21	C 2	P M	P C
C M	C C	P 2/M	P 21/M	C 2/M
P 2/C	P 21/C	C 2/C		

The point positions generated from these symbols correspond to the monoclinic setting with **b** as unique axis ($\alpha=\gamma=90^\circ$)

ORTHORHOMBIC

P 2 2 2	P 2 2 21	P 21 21 2	P 21 21 21	C 2 2 21
C 2 2 2	F 2 2 2	I 2 2 2	I 21 21 21	P M M 2
P M C 21	P C C 2	P M A 2	P C A 21	P N C 2
P M N 21	P B A 2	P N A 21	P N N 2	C M M 2
C M C 21	C C C 2	A M M 2	A B M 2	A M A 2
A B A 2	F M M 2	F D D 2	I M M 2	I B A 2
I M A 2	P M M M	*P N N N	P C C M	*P B A N
P M M A	P N N A	P M N A	P C C A	P B A M
P C C N	P B C M	P N N M	*P M M N	P B C N
P B C A	P N M A	C M C M	C M C A	C M M M
C C C M	C M M A	*C C C A	F M M M	*F D D D
I M M M	I B A M	I B C A	I M M A	

TETRAGONAL

P 4	P 41	P 42	P 43	I 4
I 41	P -4	I -4	P 4/M	P 42/M
*P 4/N	*P 42/N	I 4/M	*I 41/A	P 4 2 2
P 4 21 2	P 41 2 2	P 41 21 2	P 42 2 2	P 42 21 2
P 43 2 2	P 43 21 2	I 4 2 2	I 41 2 2	P 4 M M
P 4 B M	P 42 C M	P 42 N M	P 4 C C	P 4 N C
P 42 M C	P 42 B C	I 4 M M	I 4 C M	I 41 M D
I 41 C D	P -4 2 M	P -4 2 C	P -4 21 M	P -4 21 C
I -4 M 2	P -4 C 2	P -4 B 2	P -4 N 2	P -4 M 2
I -4 C 2	P -4 2 M	I -4 2 D	P 4/M M M	P 4/M C C

*P 4/N B M	*P 4/N N C	P 4/M B M	P 4/M N C	*P 4/N M M
*P 4/N C C	P 42/M M C	P 42/M C M	*P 42/N B C	*P 42/N N M
P 42/M B C	P 42/M N M	*P 42/N M C	*P 42/N C M	I 4/M M M
I 4/M C M	*I 41/A M D	*I 41/A C D		

TRIGONAL

P 3	P 31	P 32	R 3	P -3
R -3	P 3 1 2	P 3 2 1	P 31 1 2	P 31 2 1
P 32 1 2	P 32 2 1	R 3 2	P 3 M 1	P 3 1 M
P 3 C 1	P 3 1 C	R 3 M	R 3 C	P -3 1 M
P -3 1 C	P -3 M 1	P -3 C 1	R -3 M	R -3 C

All R-space groups refer to the hexagonal setting

HEXAGONAL

P 6	P 61	P 65	P 62	P 64
P 63	P -6	P 6/M	P 63/M	P 6 2 2
P 61 2 2	P 65 2 2	P 62 2 2	P 64 2 2	P 63 2 2
P 6 M M	P 6 C C	P 63 C M	P 63 M C	P -6 M 2
P -6 C 2	P -6 2 M	P -6 2 C	P 6/M M M	P 6/M C C
P 63/M C M	P 63/M M C			

CUBIC

P 2 3	F 2 3	I 2 3	P 21 3	I 21 3
P M 3	*P N 3	F M 3	*F D 3	I M 3
P A 3	I A 3	P 4 3 2	P 42 3 2	F 4 3 2
F 41 3 2	I 4 3 2	P 43 3 2	P 41 3 2	I 41 3 2
P -4 3 M	F -4 3 M	I -4 3 M	P -4 3 N	F -4 3 C
I -4 3 D	P M 3 M	*P N 3 N	P M 3 N	*P N 3 M
F M 3 M	F M 3 C	*F D 3 M	*F D 3 C	I M 3 M
I A 3 D				