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FRANK J. SEILER RESEARCH LABORATORY

DRAW:
Molecule Drawing
Program Version 2.00

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DRAW is a graphical program for manipulating and interpreting input and results files for MOPAC. Many common terminals and hard copy devices are supported. For manipulating the data, a machine-independent editor is provided which allows atoms to be added to a data-set, positions of atoms to be modified, atom types and connectivities to be redefined. DRAW allows molecular fragments to be added together to form larger systems. Three graphical representations of molecules are supported: line drawings, ORTEP and NAMOD. Using line drawings, the normal modes of vibrations can be displayed. The graphical representations can be rotated under user control. When used in conjunction with the program DENSITY, electron density contour maps can be generated. Geometric quantities such as bond lengths, nearest neighbors, and torsion angles can be displayed on request.

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DRAW: MOLECULE DRAWING PROGRAM
Version 2.00

JANUARY 1989

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CHAPTER 1

INTRODUCTION

1.1 BACKGROUND

The DRAW program was developed to address various needs encountered during many years of molecular orbital calculations, first using the original MNDO program (QCPE 353) and more recently the MOPAC program (QCPE 455). DRAW also works with other programs of the "MOPAC family" including DENSITY (QCPE 492) and MOSOL (QCPE 495).

The primary need was to evaluate the correctness of starting geometries prior to performing long, expensive calculations and review the resulting optimized geometries after calculation. For obvious reasons, this need was best met graphically. This need has been met by various programs, e.g. NAMOD (QCPE 370) and ORTEP (Oak Ridge Thermal-ellipsoid Plot, ORNL-5138) However, earlier programs were developed to run as batch calculations on large, centralized computer facilities which generated displays on off-line X-Y plotting devices. The user had to guess the desired orientation then wait as much as several hours to receive the output. The user repeated the process until he finally accepted "nearly perfect" display results after numerous trials.

Following the trend toward increased availability of interactive computing coupled with new, inexpensive high-resolution graphics computer terminals, DRAW attempts to prove that one picture is worth a thousand pieces of numerical data. The primary objectives during development have been (a) ease of use, and (b) simplicity of design. You have access to virtually all of the display parameters and data via simple commands. Most commands are identified by one or two letters. Commands may be entered in either upper case or lower case letters. DRAW features top-down design with a few branched modules for data input, terminal drivers, and display generation. Additional program modules can be added to accept new input file formats or different graphic terminal protocols.

The controlling logic of DRAW along with all information, rotation, moving, editing, and stick-figure drawing routines are within the public domain. The two perspective molecular modeling sections - NAMOD and ORTEP, originated from source code, originally from QCPE, but which have been adapted to merge with the structure and protocol of the DRAW program.

I have done everything possible to remove bugs from DRAW. The worst bugs, those which cause a program to end fatally, are virtually extinct. But, being realistic, in any program of this size there are bound to be a few minor errors left. I will continue development of DRAW and all reported bugs will be corrected in later versions.

1.2 GENERAL CAPABILITIES

With DRAW you can display a geometry file in any orientation. You can remove any atom or group of atoms from the picture, temporarily or permanently. Rotation commands offer a variety of methods to orient your molecule. After you find the desired orientation, the style of display can be changed to the NAMOD perspective model or to high resolution ORTEP. Additionally, you can edit the actual molecular geometry to create a new molecular geometry or even a new compound. The new molecular geometry can be used to create a new data file for subsequent calculations.

DRAW is written in standard FORTRAN-77 (ANSI X3.9-1978, ISO 1539-1980 E) so it should compile, link, and execute properly on most computers. There are still a few lines of non-standard FORTRAN code which perform functions which are convenient and can not be replaced by standard code. This is explained fully in the chapter titled "DEBUGGING DRAW".

The input modules are designed to accept input and output files from MOPAC and DENSITY. DRAW automatically recognizes the type of file. Therefore, you may call your files any name. However, DRAW was originally written for a Digital Equipment Corporation (DEC) VAX computer operating under the VMS operating system, so default file names for files that DRAW creates are standard DEC names with extensions - but you can override the file name or change the code.

Finally, except for the dual purpose HELP files, DRAW is self-contained. There is no command file to assign files. When DRAW is executed, it prompts for the name of a file, assigns it and operates automatically under your control from there on.

1.3 CHANGES FROM PREVIOUS VERSIONS

VERSION 1.00 - This was the original QCPE (QCPE 493) version of DRAW. There should not be a version with an earlier number. It was contributed to QCPE in June 1984 from Prof. M.J.S. Dewar's group at The University of Texas at Austin.

VERSION 2.00

A. Additional graphics devices supported:

   1. Retrographics modified terminals
   2. DEC VT240/VT241
   3. Tektronix 4010
   4. Epson FX-80 matrix printer
   5. DEC LA50 matrix printer
   6. MPI 99 matrix printer
   7. Hewlet-Packard color plotter

B. Display of normal modes of vibration

C. Atom labels may be assigned individually

D. Input accepts MOPAC Dynamic Reaction Coordinate (DRC) files.

E. Corrected error when deleting atoms in EDIT command

F. ORTEP drawings do not flatten atoms on the edges of the picture.

G. New or modified commands:

   1. NEXT [+]## - allows skipping ## intermediate geometries in the current input file
   2. RETRO, VT240, 4010 recognized by TERMINAL command
   3. PLOT subcommand of DISPLAY allows selecting device for off-line plotting. Recognized devices are TIGER (IDS Paper Tiger), EPSON, LA50, MPI-99, and Hewlet Packard (HP) plotters

4. VIBRATION subcommand of DISPLAY selects vibrational mode to display

5. LABEL subcommand of DISPLAY

6. MAP subcommand of DISPLAY shows terminal color map

7. MERGE subcommand of EDIT merges geometry descriptions

8. RADIUS subcommand of INFORMATION searches for neighboring atoms within a specified distance

H. Change in terminology for NAMOD perspective drawings.

1.4 DRAW REFERENCES

Users are encouraged to reference DRAW in their publications. The reference should cite the QCPE program number 493 and the version of DRAW. DRAW, Version 2.00, Quantum Chemistry Program Exchange, Department of Chemistry, Indiana University, Indiana 47405, No. 493, written by Donn M. Storch.

1.5 ACKNOWLEDGEMENTS

A program of this size is rarely created with no external help. The following people or institutions have been instrumental in the development of DRAW.

1. The U.S. Air Force for sponsoring my Ph.D. program,

2. Prof. Michael J.S. Dewar who directed my Ph.D. program, of which DRAW later became a part,

3. The Department of Chemistry at the USAF Academy for allowing me the time to improve DRAW,

4. The Frank J. Seiler Research Laboratory (AFSC) also at the USAF Academy, for the computer time and storage to work on DRAW,

5. Dr. James J.P. Stewart for advice, editing and general ideas. Jimmy wrote the original version of subroutine READER,

6. The late Dr. Gilbert Grady, St. Michaels College, for numerous suggestions and assistance on the GIGI terminal driver,

7. Dr. James Freidheim for his patience in the initial debugging efforts with the EDIT command,

8. Dr. Y. Beppu who was kind enough to provide documentation of the NAMOD perspective program which I had earlier called the NAGOYA representation.

9. Captains Herb Klei and Jon Swanson (FJSRL) for their suggestions and improvements in 'porting' DRAW,

10. And numerous students and colleagues for suggestions and advice on what to do with DRAW.

Thank you.

CHAPTER 2

RUNNING DRAW

2.1 INSTALLING DRAW

Before running DRAW someone has to install it on a computer.

Installing DRAW is covered in chapter 8. This includes putting together the source to create an executable image, creating a HELP library (on a VAX computer), and assiging logical names and symbols to run DRAW from a central directory. If you are the first person on your computer to have DRAW, you will have to go through all of chapter 8. However, if someone else has DRAW running on your computer, the two of you (with some help from the system manager) can use the one copy. You will still have to create the operating system pointers so you can find and execute the program.

2.2 OPERATING DRAW

DRAW is designed to run interactively. You will interact with the program in a flexible manner. When started, DRAW initializes certain data areas to allow all symbols except dummy atoms (symbol XX) to be drawn. The terminal type is set to NON-GRAPHIC with ZERO lines of text on the screen. Display style is set to draw STICK figures with atom positions LABELED with the NUMBER of the atoms. I have chosen these default settings because they provide the most rapid format of interaction for the widest range of uses. You can select your display parameters easily before beginning the slower process of drawing molecules. (See figure 1.)

DRAW next asks you to enter the name of the input file:

```
What is name of file [.ARC]
```

Because ARCHIVE files from MOPAC are the most commonly examined files, the default extension for the file name is ".ARC". DRAW asks this question whenever it needs a new input file name. If you press the carriage return without entering a name, DRAW QUITS. If your response is a question mark "?", DRAW provides HELP. Any other response is interpreted as a file name. Thus, the response

G

will cause DRAW to attempt to open "G.ARC" for input. If you wish to draw a file with any other extension, you should include the extension as part of the file name. E.g., "METHANE.DAT" will override the default .ARC extension causing DRAW to attempt to open "METHANE.DAT" for input.

If your input file does not exist, you will be warned, but DRAW will then prompt for commands in a normal manner. Of course, certain commands will not function if there are no atoms in the geometry. However, in this way, you can create a geometry description from scratch using the EDIT functions.

The functions of DRAW's commands are covered in the next chapter. They are arranged alphabetically with sub-commands entered under their principal command.

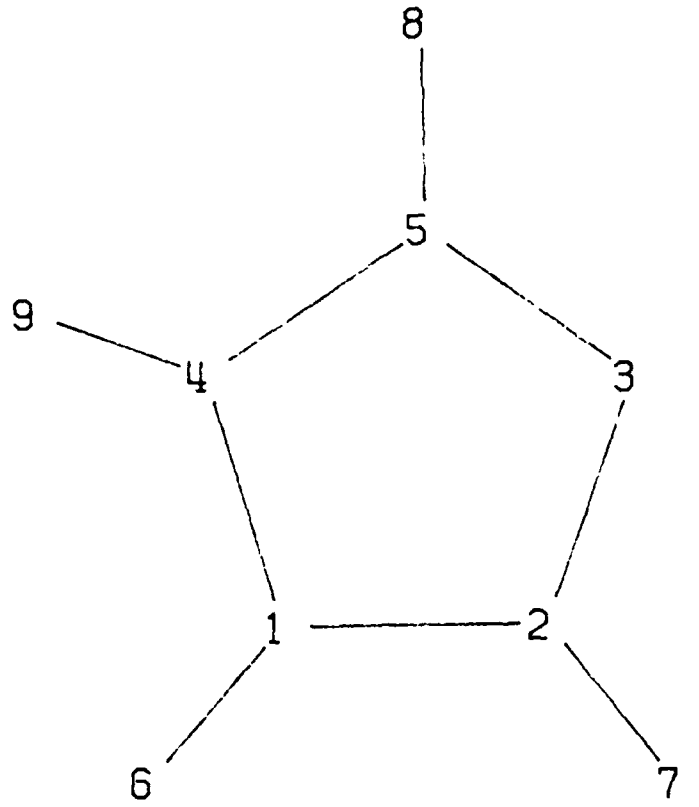

Figure 1. Imidazole shown with default settings.

CHAPTER 3

COMMANDS

In general, DRAW responds to simple English language commands. Usually, you need enter only enough letters of the command to distinguish it from other commands at that level of the program. Some of the DRAW commands are divided into groups under a higher level command. For example, under ROTATE there are seven sub-commands controlling the type of rotation and the application of the rotation. The hierarchy of commands is indicated in the following manner. When DRAW is ready for a command, it will prompt with

```
DRAW>
```

I call this prompt the "top-level" prompt because it comes from the highest or top level of DRAW. At this point, any top-level command, e.g. ROTATE, may be entered. If the command does not have subcommands, DRAW will execute the command immediately. However, if, as in the case of ROTATE, there are subcommands available, and you have not specified the subcommand to use, the ROTATE command will prompt as

```
Draw: ROTATE>
```

to indicate that the next command entered will be interpreted as a subcommand of ROTATE.

In DRAW some commands have optional arguments. In this manual, such options are identified in special ways:

```
Plot [integer] [<file name>,*]
```

In the above example, [integer] is an optional integer. Also, [<file name>] represents an optional file name (which should be compatible with your computer's file names) and [*] represents an alternate, optional reference for the file name.

You may enter more than one command per line. Each command will be executed sequentially. For example:

```
ROTATE CARTESIAN 2 30.0 45.0 0.0
```

will cause the molecule to be rotated about atom 2 by 30.0 degrees about the X-axis and 45.0 degrees about the Y-axis. Whereas,

```
I N Q
```

will cause DRAW to enter the INFORMATION command level, search for and print the two NEAREST atoms and then QUIT back to the top level.

3.1 BELL

Causes the terminal bell to ring when the program is ready for a new top level command. If you enter B (not BELL), the bell will ring only the one time. The main use for this command is in drawing large, detailed pictures where the user may not be at the terminal while the picture is being drawn.

3.2 COMMAND

Allows you to store one line (approximately 70 characters) of commands. These commands will be executed after each NEXT geometry is drawn. To erase (and de-activate) the stored commands, type "QUIT" in response to the COMMAND prompt. The primary use of this facility is in examining successive geometry descriptions in a file from a reaction path calculation. The stored commands can automatically monitor the calculated heat of formation or a specific interatomic distance, bond angle or dihedral for each geometry in the path. This function is available as a result of the cohesive nature of DRAW. Generally, you can "run" many commands together on a single line.

3.3 DISPLAY

** NOTE: You must use the QUIT subcommand to leave the DISPLAY command. The changes requested via subcommands of DISPLAY will be made after you QUIT.
See the QUIT subcommand.

Enters the DISPLAY mode. In this mode, you can select or modify parameters associated with the picture displayed or printed. All of the display commands affect each of the three display styles, STICK FIGURES, NAMODI, and ORTEP, in the same manner. While you are in the DISPLAY command, the prompt from DRAW will be

DRAW:DISPLAY>

which will remind you what type of commands are permitted.

1) +## Allows the drawing of any specific atom. To allow atom number 9, use +9. This subcommand works on any atom regardless of atomic symbol. This command DOES NOT ADD new atoms to a geometry description; it allows existing atoms to be drawn in the picture. The default setting in DRAW is that all atom numbers are allowed. See the corresponding "-##" command and the similar +SS and -SS commands. The interaction between the +/-## and the +/-SS commands are that an individual atom must be allowed by both. This is a logical AND function.

2) -## Masks the drawing of any specific atom. For example, -9 prevents the display of atom number 9 of the molecule. The atom is not removed from the molecule; it is simply not drawn in the current picture. This subcommand works on any atom regardless of atomic symbol. The default setting in DRAW is that all atom numbers are allowed. See the corresponding "+##" command and the similar +SS and -SS commands. The interaction between the +/-## and the +/-SS commands are that an individual atom must be allowed by both. This is a logical AND function.

3) +SS Allows the display of certain elements. To allow drawing of all hydrogen atoms, type +H. This command WILL NOT ADD new atoms to a geometry; it simply allows existing atoms to be drawn. Similarly, +XX (here, XX is a type of atom called a dummy atom) will allow all dummy atoms to be drawn. The default in DRAW is -XX and all other atoms are allowed. See the corresponding -SS command and the similar +## and -## commands. The interaction between the +/-## and the

+/-SS commands are that an individual atom must be allowed by both. This is a logical AND function.

4) -SS Masks the display of certain elements. For example -H prevents the display of all hydrogen atoms. The atoms are not removed from the molecule; they are simply not drawn in the current picture. The default in DRAW is -XX (here, XX is a type of atom called a dummy atom) and all other atoms are allowed. See the corresponding +SS command and the similar +## and -## commands. The interaction between the +/-## and the +/-SS commands are that an individual atom must be allowed by both. This is a logical AND function.

5) BONDS Selects and modifies the criterion by which bonds are selected to be drawn. The default is RADIUS times 1.4.

1. BONDORDER If the input file contains bond-order information, DRAW will use it to select bonded atoms. When you start reading a new input file, DRAW will decide automatically whether to use the BONDORDER matrix if it finds bond-order information in the input file.

2. RADIUS If two atoms are within 1.4 times the sum of their covalent radii, they are connected by a bond. When a file is first read, DRAW will decide AUTOMATICALLY whether to use BONDORDER matrix or RADIUS depending upon whether it finds bond-order information in the input file.

3. MANUAL You can override the bond selection of DRAW. You can erase selected bonds or create bonds. DRAW will start with the current set of bonds whether from the BONDORDER matrix or RADIUS. You can then alter the set of bonds. You create a bond by entering the numbers of the two atoms to bond. DRAW will not check whether the bond allready exists or whether the bond makes sense. To remove bonds, simply make one of the atom numbers negative. E.g., 5,9 will connect atoms 5 and 9 while -5,3 will remove the bond between atoms 5 and 3. You can also remove all bonds to an atom: -12,* will remove all bonds to atom 12. DRAW will not check whether the specified atoms were bonded originally.

6) COORDINATES You may select the number of cartesian coordinates displayed on the right hand side of your terminal. For PLOT style output devices this command will not affect the coordinate output. Printer style devices will print all coordinates while X-Y devices will not list any. You may use this command to display coordinates on a non-graphic terminal.

7) HELP Typing H or ? will enter the HELP facility. Once in this facility, you can obtain help information for this command level or any other DRAW command or subcommand. For more information on using the HELP facility, see the HELP command in this chapter.

8) LABELS Select or remove type of labels used in picture. The default is NUMBER where the label is the number of the atom in the molecule. (See figures 1 and 2.)

1. SYMBOL uses atomic symbols to label the position of atoms.

2. MASK prevents drawing of labels for all atoms. This mode is represented differently in the different display styles. For STICK drawings, hydrogens are not drawn and carbons are only sticks or junctions of bonds. This style is chosen to approximate an organic chemist's idea of line drawings. In NAMODI, atom circles are drawn with no symbols at all. In ORTEP, all atoms are drawn but with the cross hatching commonly seen in ORTEP style pictures.

3. BOTH creates labels with the atomic symbol and the atom number.

4. USER allows you to enter individual labels for each atom. This may be tiresome for large molecules but DRAW does offer a default for each atom in the format of BOTH atomic symbols and atom numbers. If you use this subcommand for ORTEP drawings and specify a blank label, atoms will be drawn with only a circle: there will be no perspective cross on the atom.

There is one difference in the action of this subcommand on ORTEP drawings. If you want "normal" ORTEP drawings which have contour lines crossing the elipsoids, MASK labels.

9) MAP Will display the color map for elements in the current geometry display. Next, if your terminal does not support color or (more likely) if DRAW does not support color for your terminal, DRAW will tell you that color is not supported. If color is supported, DRAW will tell you and give you an opportunity to turn it off. This may be desired if you are making hard copies directly off the screen and do not wish to have colors. If you keep the colors, you will be asked if you want to alter the color map. DRAW's idea of colors is:

MAP NUMBER	COLOR
1	WHITE
2	GREEN
3	RED
4	YELLOW
5	BLUE
6	CYAN
7	MAGENTA
8	ORANGE
9	GREEN-YELLOW
10	GREEN-CYAN
11	BLUE-CYAN
12	BLUE-MAGENTA
13	RED-MAGENTA
14	DARK GRAY
15	LIGHT GRAY

You may alter the color that are used to represent any element in your current geometry description or any other element. The above listing does not include BLACK which some terminals call the background color. If your terminal does not support 15 colors, DRAW will use some sub-set of the above colors. Every attempt is made to use distinctive colors.

There is no way to interactively alter the color map.

10) NAMODI Selects the NAMODI style of perspective drawing where atoms are drawn as circles with radii based on covalent radii and distance from the XY plane. Bonds are drawn with taper indicating perspective. The rate of drawing is intermediate between STICK and ORTEP. This style was mistakenly called NAGOYA in the previous version of DRAW.

11) ORTEP Selects the Oak Ridge Thermal Elipsoid Plotting style. Atoms are drawn as circles (no thermal uncertainty). Bonds are drawn as tapered rods. This is a slow method of drawing but produces high quality perspective drawings. See the note on the LABELS subcommand regarding ORTEP representation of atoms. (See figure 3.)

12) PLOT Allows you to chose the type of off-line plotting device for which a file is created by the PLOT command of DRAW. The default device is an EPSON FX-80. Your choices include various bit-mapped matrix printers and X-Y plotters.

1. CALCOMP - Creates a plotting command file for a CALCOMP M84 plotter. This will support different colors.

2. EPSON - This creates a file which may be directly printed on an EPSON FX-80 matrix printer. No color selection is available.

3. HP - Will create a file which may be written to any XY plotter which supports the HPG graphic language. DRAW only uses a limited (i.e., small) subset of the HPG language. This plotter style supports colors.

4. LA50 - Creates a file which may be printed on a DEC LA50 matrix printer. This file makes use of the LA50 data compression capability so printing it at low data transfer rates is not impractical. This code also works on a DEC Letterwriter IV. No color selection is available.

5. MPI-99 - A dot matrix printer built by the MPI corporation. No color selection is available.

6. TIGER - This refers to an IDS PAPER TIGER printer. No color selection is available. This was the only device supported in version 1.00.

13) QUIT Leave the DISPLAY modification logic. The picture is re-drawn and will reflect all changes. Note that none of the changes requested in DISPLAY will take effect until AFTER you QUIT.

14) SCALE You may alter the amount of display area used by the plotting routines. This command will show the current scale factors for hard copy (H=) and for CRT (C=). The values are altered by specifying which one to change (eg. C=30 will draw pictures on the CRT which are 30% of the original size.) Changes made in the scaling are retained until specifically altered (see PLOT command at the top level.)

15) STICK Selects STICK style of drawing. Atoms are shown by label (if labelling is enabled) only and bonds are single lines. No perspective is shown. This is the default mode and is the fastest mode of drawing. I suggest using the STICK mode to find the desired perspective and then switching to another mode for the final drawing.

16) TITLE You may input up to 80 characters to use as a title for any style displays. The default title is blank for STICK or NAMODI representations. The default title is the file name for ORTEP representation.

17) VIBRATION Display of normal modes of vibration is available for STICK drawings only (at this time.) The normal modes are identified by an integer which describes their energy order as produced in a MOPAC output file resulting from a FORCE calculation. The default mode is number 1. For motions which are largely in the plane of the drawing, the motion is represented by an arrow showing the direction and magnitude of the mass-weighted motion of each atom. If the motion is primarily out-of-plane, the motion is represented by either an X for motion in the positive Z-direction (i.e., toward you) or by a circle with an X for motion in the negative Z-direction. The motion indicators will transform as you rotate the molecule. If you would rather show the direction of motion in the opposite direction, specify the NEGATIVE of the mode number. E.g., if you request -5, mode 5 will be drawn showing atom movement in the opposite direction. (See figure 4.)

If you request MODE 0 (zero), vectors will NOT be drawn. The "normal" style of drawing will be restored.

DRAW will place the molecule in the orientation used by MOPAC when the FORCE calculation was done. After you QUIT the DISPLAY command you can rotate your molecule

with the vectors to any orientation you want. Each time you select a new vibration mode or phase, DRAW will return the molecule to the orientation MOPAC used for the FORCE calculation.

18) ZOOM Allows you to select certain atoms or a portion of the entire molecule to display. This is an automatic feature similar to +/-##. You may select atoms to be displayed MANUALLY, by entering the atom numbers, by automatically selecting all atoms which are allowed to be OPTIMIZED, or you may select a SURFACE of atoms. The SURFACE is always parallel to the X-Y plane. (The X-Y plane is parallel to the screen of your terminal.) Once you select a surface, you can select the next adjacent surface above (+) or below (-) the current surface, or you can show the TOP or the BOTTOM of the molecule.

3.4 EDIT

** NOTE: You must use the QUIT subcommand to get out of the EDIT command. See the QUIT subcommand.

Edit provides access to all components of the geometry description. You can change any coordinate of any atom in the geometry. In addition, you can add new atoms to the end of the geometry description and remove atoms from the end.

While you are in the EDIT command, the prompt from DRAW will be

DRAW:EDIT>

which will remind you what type of commands are permitted.

1) ## This is the default mode of operation in EDIT. Atoms are selected to be changed by simply typing the number of the atom whose coordinates you wish to change. If you type only the number of the atom, DRAW will display the current coordinate description of the atom. Any part of the geometry may be changed by typing the atom number followed by a command letter and the new value, e.g.:

4 B 1.3 - will set a new bond length of 1.3 Angstrom between atom 4 and the atom to which atom 4 is related via the current internal coordinate description.

You may combine all of the changes for any atom on one line of input:

4 B 1.3 NA 2 NB 3 will alter the bond length and change the connectivity so the bond length reference atom is atom 2 and the angle reference atom is atom 3. If any of the changes are invalid, none of the changes will be made.

** CAUTION: The type of coordinate is set by the MODE command.

a) TYPE Will change the Type (symbol) of the selected atom. This sub-command may be used with either setting of the MODE sub-command.

b) ANGLE Changes the bond angle as specified in the current internal coordinate description. Internal mode must be set to use this sub-command.

c) BOND Will change the bond length as specified in the current internal coordinate description. Internal mode must be set to use this sub-command.

d) DIHEDRAL Changes the dihedral angle as defined in the current internal coordinate description. You must set the mode to internal to use this sub-command.

e) IA Change the optimization flag for the angle coordinate. A "0" here will prevent this parameter from being optimized in MOPAC. A "1" allows optimization; while a "-1" identifies this coordinate as a reaction path.

f) IB Change the optimization flag for the bond coordinate. A "0" here will prevent the this parameter from being optimized in MOPAC. A "1" allows optimization; while a "-1" identifies this coordinate as a reaction path.

g) ID Change the optimization flag for the dihedral angle coordinate. A "0" here will prevent the parameter from being optimized in MOPAC. A "1" allows optimization; while a "-1" identifies this coordinate as a reaction path.

h) NA Change the atom to which the distance coordinate refers. This sub-command may be used with either setting of the MODE sub-command. If your new value for NA is invalid (either greater than the number of the current atom or equal to NB or NC) the value will not be changed. If you wish to change NA and one or more of the other reference atoms, enter all changes on one line:

NA 5 NC 3 which will change both references before checking the validity.

i) NB Change the atom which specifies the terminus of the angle coordinate. This sub-command may be used with either setting of the MODE sub-command. If your new value for NB is invalid (either greater than the number of the current atom or equal to NA or NC) the value will not be changed. If you wish to change NB and one or more of the other reference atoms, enter all changes on one line:

NA 5 NB 3 which will change both references before checking the validity.

j) NC Changes the atom which specifies the end of the dihedral coordinate. This sub-command may be used with either setting of the MODE sub-command. If your new value for NC is invalid (either greater than the number of the current atom or equal to NA or NB) the value will not be changed. If you wish to change NC and one or more of the other reference atoms, enter all changes on one line:

NA 5 NC 3 which will change both references before checking the validity.

k) X Alters the X coordinate of the selected atom. Cartesian mode must be set to use this sub-command.

l) Y Alters the Y coordinate of the selected atom. Cartesian mode must be set to use this sub-command.

m) Z Alters the Z coordinate of the selected atom. Cartesian mode must be set to use this sub-command.

n) DUMMY Insert a DUMMY atom (symbol "XX") at any point in the current geometry description.

o)

EDIT N Allows you to edit the three lines of text from a MOPAC data file. "E 1" will display the KEYWORD line and ask whether you want to REPLACE or SUBSTITUTE the text in the line. If you chose REPLACE, DRAW will read the next line you type and will place it in the file as the new KEYWORD line. For small changes, on the other hand, you can SUBSTITUTE. To use SUBSTITUTE you enter

S/old text/new text/

The "/" can be any delimiter you wish to use. DRAW will replace the first match of "old text" with "new text". The "new text" part can be longer or shorter that the "old text" part. For example,

S/FRED//

will remove the string "FRED" and replace it with nothing.

p) HELP Typing H or ? enters the HELP facility. Once in this facility, you can examine help information from this command level or any other DRAW command or subcommand. For more information on using the HELP facility, see the HELP command in this chapter.

q) INFORMATION Enters the information routine directly to allow evaluation of editing changes. See the section on INFORMATION for more information.

r) MERGE In response to the MERGE subcommand, DRAW prompts for the name of a file to read:

What is the name of file [.DRW] ?

DRAW will open and read the specified file using exactly the same logic by which it reads the normal input file. You can MERGE any type of file that DRAW recognizes (see chapter 6, "DRAW FILES".)

If there are no atoms in the current geometry description before your MERGE command, the new file will be brought in directly with no additional information needed. If there are some atoms in the

current description, you will have to supply some of the "missing" internal coordinates. The new file will lack six internal coordinates:

Atom 1	-	distance, angle, dihedral
Atom 2	-	angle, dihedral
Atom 3	-	dihedral

You will have to provide some or all of these along with the reference atom(s) NA, NB, and NC. These reference atoms, of course, must be part of the current (original) geometry description that was present before merging.

After you supply the necessary internal coordinates, DRAW will actually join the new geometry to the current geometry. If you have a graphic terminal, the new section will be displayed (subject to the usual constraints of screen clipping, etc.)

s) MODE This sub-command accepts two arguments:

a) INTERNAL Tells DRAW to accept commands which affect INTERNAL COORDINATES only. Such commands usually identify which coordinate type is expected by the syntax of the prompt. (See the "+" command in this section.)

b) CARTESIAN Tells DRAW to accept commands which affect CARTESIAN COORDINATES only. Such commands usually identify which coordinate type is expected by the syntax of the prompt. (See the "+" command in this section.)

The setting of MODE affects the action of the "##" command as well as the "+" command.

t) + This is a powerful method of building complex structures. Typing "+" causes the program to prompt for the coordinates of a new atom. If INTERNAL COORDINATES are expected (see the MODE command in this section) the prompt will be as:

IC of atom 23:

If, however, CARTESIAN COORDINATES are set:

CC of atom 23:

The setting of the MODE command controls whether "+" accepts Internal or Cartesian coordinates. The new atom number will be N+1; i.e., the new atom will be placed at the end of the geometry description. You must specify the values of NA, NB, and NC, even for cartesian coordinates. Data input is free format, as is most of DRAW, and must contain: Atomic symbol, Distance, Angle, Dihedral, NA, NB, NC. If you wish, you may also include the optimization codes for the internal coordinates. Each new atom entry is scanned for errors before being added to the geometry description. On a graphic terminal, the new atom will be drawn in its proper place unless the position is beyond the viewing area of your screen. Any potential bonding interactions between the new atom and previous atoms will be drawn. Then each atom in the geometry description will be re-evaluated to see if the number of potential bonds exceeds the "normal" valency. You will be notified of any violations.

** NOTE: Pressing the carriage return on an empty line will cause the ADD mode to quit.

Be sure to use the OUTPUT command to create a new file with the new geometry description before you QUIT DRAW.

2) -## Typing "-##" causes the ## numbered atom to be deleted from the geometry description. It is actually removed (as opposed to the action of commands in DISPLAY.) If ## is not specified the highest numbered atom in the geometry description is deleted. If the specified atom is used as a reference for a subsequent atom in the description, DRAW will tell you and will refuse to delete the atom. Before you can delete the atom, you must alter the later atom which refers to it (by setting the MODE to cartesian and by changing the reference entry). The only atoms which cannot be deleted are the first three atoms in the description. If you must delete one of these, the easiest method is to change the atom type to DUMMY (symbol XX).

The action which DRAW uses to delete an atom depends upon whether you are deleting the last (terminal) atom of the current geometry description, by the "-" command or some other atom, "-##". A terminal atom is actually removed from the geometry description at the same time that it is erased from the display. The number of atoms

in the description is reduced by one. It is as though the atom never existed.

```
*******************************
 THIS ACTION IS IRREVERSIBLE.
*******************************
```

On the other hand, if you delete any atom other than the terminal atom, DRAW will "mark it for deletion". Actually DRAW changes the type of atom to "DD". (DO NOT do this yourself with other editor functions - this would cause severe problems.) DRAW checks whether any subsequent atom in the description explicitly refers to the atom you want to delete. If any do, DRAW warns you and will not mark the atom for deletion. The atom is not removed from the description until you QUIT the EDIT function.

```
*******************************
 THIS ACTION IS REVERSIBLE.
*******************************
```

If you alter the atom TYPE so it is NOT "DD", it will not be deleted when you QUIT the EDIT function.

3) PICTURE During normal operation, EDIT does not re-scale the display. As a result, some changes to a geometry may place an atom beyond the edge of the display area. When this happens DRAW will clip (or truncate) that portion of the picture. PICTURE will cause the current geometry description to be re-drawn.

4) QUIT This is the only way to get out of the EDIT command. If you have made any editing changes, DRAW will re-draw the picture. This is done to re-adjust the graphic parameters to allow sufficient borders for subsequent DRAW activities.

3.5 GIP

Command: GIP [<filename>] [##]

This command produces a special GIP (Geometry Interchange Program) file. The file will be named <filename>.GIP and can be edited via any text editor. The optional argument [##] causes all of tne internal coordinate references, NA, NB, and NC, to be

offset by the number of the argument. E.g., GIP 5 will cause five to be added to each internal coordinate reference. This is handy for off-line (i.e., outside of DRAW) merging of files. If you wish to combine two separate molecular files containing, for example, 5 and 8 atoms, you could create a GIP file of the larger molecule with an offset of 5 atoms. This file could then be added to a GIP file (with offset of zero) of the smaller molecule. The resultant file may require some minor editing but most of the reference atoms will be correct. See the chapter titled "GEOMETRY INTERCHANGE PROGRAM".

3.6 HELP

Typing H or ? will enter the HELP facility. Once in this facility, you can examine help information for this command level or any other DRAW command or subcommand. The HELP facility works similarly to the DEC VMS help facility. Once in the facility, you may move up or down the hierarchy of commands and subcommands to find any information. You move down the help structure by typing a topic of interest from the listing of available topics. Topics are recognized by entering enough letters to identify the topic uniquely. You move up the help structure by pressing the carriage return without entering a topic. The prompt format tells how far down the help structure you have gone. For example,

```
HELP: DRAW:
```

is the highest level in the help facility. While

```
HELP: DRAW: ROTATE:
```

is one level down in the help facility. You exit HELP by moving up the help structure above the highest level.

** NOTE: Do not use QUIT to leave the HELP facility. Exit HELP by moving up the help structure above the highest level. Simply press return a number of times until you have exited the facility. If you do type QUIT, the HELP facility will explain how the QUIT command works.

The information available through HELP is contained in a separate file "DRAW.HLP". This separation of help text from the executable provides easier maintenance of both the executable

code and the help information. The file DRAW.HLP can be used by VAX users to construct a help library which is available to users via the VAX VMS help facility.

The source file, "DRAW.HLP", can also be used by MOHELP (QCPE 454). Indeed, MOHELP is actually the same subroutine as DRAW's HELP function but written as a stand-alone function capable of reading other help files.

3.7 INFORMATION

** NOTE: You must QUIT to get out of INFORMATION.
See the QUIT subcommand.

This section provides information about the molecular description and the input file.

While you are in the INFORMATION command, the prompt from DRAW will be

DRAW:INFORMATION>

which will remind you what type of commands are permitted.

1) ## This is the normal mode of the INFORMATION command. The basic mode of this routine is geometry. The routine can provide:

##	- atomic symbol, cartesian coordinates and bonded neighbors
##,##	- distance between the specified atoms
##,##,##	- angle described by the three atoms
##,##,##,##	- dihedral described by the four atoms

Eg. 5,21,3 will report the angle described by the three atoms. The atoms do not have to be connected in any way. ATOM NUMBERS MAY ALSO BE SEPARATED BY SPACES.

2) BOND ORDER If the input file has a bond order matrix, it is printed.

3) COUNT Prints the number and types of atoms (including dummy atoms), the number of orbitals and number of electrons and the chemical formula.

4) FILES Lists the names of files used for input. Output files are not created until the proper commands are entered; e.g., OUTPUT, PLOT, GIP, etc.

5) HELP Typing H or ? will enter the HELP facility. Once in this facility, you can examine help information from this command level or any other DRAW command or subcommand. For more information on using the HELP facility, see the complete HELP command described earlier in this chapter.

6) INFORMATION Prints the first three lines of the input file (if internal geometry or archive). If the input file is an archive or output type, DRAW will list various calculated values: Heat of formation, IP, dipole, reaction coordinate, reaction coordinate gradient, and gradient norm. If the input file is from a dynamic reaction coordinate (DRC) calculation of MOPAC, DRAW will list the associated energies with the current point.

7) NEAREST Prints the numbers and separation of the two closest atoms in the molecule. Dummy atoms are not included.

8) QUIT This is the only way to leave the INFORMATION command. Since nothing in INFORMATION alters the screen display (except HELP), DRAW will not re-draw the picture. You will return to the level from which you called INFORMATION.

9) RADIUS Searches a sphere with radius you specify. Prints all atoms in order of increasing distance from the atom at the center of the sphere.

RADIUS ## [distance] [Atomic symbol]

The default radius of search is 5.00 Angstroms. If you specify an atomic symbol, only atoms of that type which are within the radius will be reported.

10) SYMMETRY If the input file had user specified symmetry relations, they are printed.

11) VALENCE Prints all atoms which have more than the normal number of bonded neighbors. The selection of bonded atoms is described in the BOND subcommand under the DISPLAY command.

3.8 LAST

Undoes the last rotation. This command will not extend backward beyond an EDIT session. See the ROTATE command.

3.9 MOVE

Allows movement of any or all atoms in cartesian or internal space. The choices of movement include:

1. CARTESIAN You can specify movement of all atoms by cartesian coordinates

2. INTERNAL COORDINATES You can specify movement of all atoms by internal coordinates

Once you have chosen the coorinate base by which you will specify the movement, DRAW will prompt for more information. If you request CARTESIAN coordinates you can move the entire molecule or individual atoms. If you want to use the Geometry Interchange Program (GIP) method to combine files, this sub-command can position the whole molecule in 3-D space to be combined with another file. Look at the chapter on GIP.

If, on the other hand, you use INTERNAL coordinates you can specify the movement as a function of a NORMAL MODE of vibration which is produced from a MOPAC force calculation. Every atom can be moved according to the normal vibration modes. DRAW will ask for the normal mode to use. Movement can be positive or negative. Of course, the input file MUST contain normal modes for this feature.

3.10 NEXT

Command: Next [Reset] [+[##]]

The program will attempt to read another geometry description from the current input file. If the end-of-file is encountered, you will be prompted for a new file name. The command

NEXT RESET

will clear all rotation information from the current geometry and read the next entry in the same input file. If RESET is not used the next geometry will be drawn with the same rotations as are currently in effect. The option +## will cause DRAW to skip over ## intervening geometry descriptions while omitting the + will cause DRAW to read forward to point ## in the current file. These options are primarily for use with the output from a MOPAC DRC calculation. If there are not ## calculation points remaining in the input file, DRAW will encounter the end of the file and will ask for the name of a new input file.

3.11 OUTPUT

Command: Output [<filename>[.DAT],*]

The program will write a file suitable for input to MOPAC. The first three lines of the file will come from the original input file. The internal coordinate description will reflect all changes made using MOVE, ROTATE or EDIT commands. Specifying a file name will override the default name. Specifying * for the file name will use the default file name but ignore any directory or subdirectory prefixes.

3.12 PLOT

Command: Plot [scale integer] [<filename>[.PLT],*]

The program will write a file which can be printed on the type of off-line device selected by the PLOT subcommand of the DISPLAY command. The file will produce a picture which reflects

the current display options in effect. The file IS NOT immediately dispatched to the printer. SCALE INTEGER is the percent of full page to be to be used by the picture (default is 100%). Specifying a file name will override the default name. Specifying "*" for the file name will use the default file name but ignore any directory or subdirectory prefixes.

3.13 QUIT

Exits the program and restores the terminal (if necessary) to non-graphic operation. If you have made any changes to the geometry via rotations of groups of atoms, or movement of groups of atoms, or by editing the description, the program will not allow you to exit without giving you a chance to save the modified geometry with the OUTPUT command.

3.14 REFLECT

Format: REFLECT [XY,XZ,YZ,INVERT]

Performs a reflection about the specified plane (XY, YZ, XZ). this occurs about the absolute coordinate plane, not relative to the molecule.

3.15 RESET

Causes all rotation information to be cleared and the molecule to be re-drawn from the internal coordinates.

3.16 ROTATE

Allows rotation of any or all atoms of a molecule. Rotations

follow the right hand rule. That is, if you place your right hand so that your thumb is pointing in the direction of the vector of rotation, positive rotation is the direction your clenched fingers curve. As viewed from the base of the thumb, positive rotation is clockwise. Negative angles of rotation are allowed.

NOTE: You may have to QUIT the ROTATE command.

While you are in the ROTATE command, the prompt from DRAW will be

DRAW:ROTATE>

which will remind you what type of commands are permitted.

1) CARTESIAN Performs the specified rotation about the three CARTESIAN axes centered on the specified atom. In the display, the positive X direction is toward your right, positive Y is toward the top of the screen, and positive Z is out of the screen toward you.

Input: ATOM NUMBER, X (degrees), Y (deg), Z (deg)

2) EULERIAN Performs the specified rotation by the three Euler angles about the specified atom.

Input: ATOM NUMBER, THETA (degrees), PHI (deg), PSI (deg)

3) GROUP You may specify any atoms in the molecule to be rotated. No information is requested until the type of rotation is started, then the program will ask for a listing of the atoms to be rotated. Rotation of a methyl group could be done in the following manner: (prompts and messages from the DRAW program are represented in capital letters while user responses are represented in lower case text and by numbers.)

```
DRAW: ROTATE> group
GROUP SET.
DRAW: ROTATE> pair 4,5,35
INPUT LIST OF ATOMS TO MOVE: 7,8,9
DRAW: ROTATE>
```

The above example would rotate a methyl group (carbon atom 5 with hydrogen [illegible] 8, and 9 which is bonded to atom 4) by 35 degrees about the bond.

4) HELP Typing H or ? will enter the HELP facility. Once in this facility, you can examine help information from this command level or any other DRAW command or

subcommand. For more information on using the HELP facility, see the HELP command in this chapter.

5) NOGROUP This will clear the GROUP request indicating that the whole molecule is to be rotated. This is the default action of ROTATE.

6) PAIR The rotation is performed about the vector defined by any two atoms. The first atom specified is the start of the vector and the second atom indicates the direction of the vector.

Input: ATOM NUMBER, ATOM NUMBER, ROTATION (degrees)

For example, 5,9,25 will rotate the molecule about the vector from atom 5 to atom 9. Applying the right-hand rule would place the thumb toward atom 9. The molecule will be rotated 25 degrees in the direction your fingers curl.

7) QUIT Exit the ROTATE command and return to the top-level of DRAW. If any rotation commands have been entered, the picture will be re-drawn. In many instances, you may wish to do only one rotation of the whole molecule. If the rotation command is entered on ONE LINE from the top level prompt, the rotation is performed and DRAW returns to the top level, e.g.

DRAW> ROTATE CARTESIAN 2,45,0,0

will rotate the entire molecule by 45 degrees about the X axis and automatically exit the ROTATE command.

3.17 SYMMETRY

The principal moments of inertia are calculated and the molecule is re-drawn with the following orientation:

Center-of-mass at the origin of the Cartesian coordinate system

Principal axis in Z direction (out of screen),

Second axis in X direction (towards the right)

3.18 TERMINAL

For additional information on TERMINALS and the method of terminal support, refer to the chapter titled "TERMINAL SUPPORT".

The type of terminal may be selected as via any of the following commands:

1) GIGI DRAW provides support for the Digital Equipment Corporation GIGI graphic terminal. Not all of the code is tested.

2) HELP Typing H or ? will enter the HELP facility. Once in this facility, you can examine help information for this command or any other DRAW command or subcommand. For more information on using the HELP facility, see the HELP command in this chapter.

3) NON-GRAPHIC Any terminal which is incapable of displaying point graphics, e.g. H-19, VT-52, VT100, ADM-31, any generic terminal emulator running on a personal computer, or any graphic terminal not yet supported by DRAW.

4) RETRO For a RETRO-GRAPHICS enhanced VT-102 terminal.

5) TERAK TERAK 8600 color terminal as supported at the United States Air Force Academy. This routine issues calls to a unique graphics routine library. Since the average user will normally not have these routines, DRAW has "dummy" routines to satisify linker calls but which do not actually perform graphics. However, since these calls conform to the ACM Graphics Core standard, users who have similar local software libraries may be able to adapt this routine to their own use.

6) TK4010 Tektronix model 4010 graphics terminal (no options are assumed.) The screen storage aspect of this terminal make it rather unsuitable for the EDIT function, but all other facilities of DRAW will work properly.

7) TK4025 Tektronix model 4025 graphics terminal (no options are assumed.)

8) TK4105 The TK4105 driving routine knows commands for the 4105, 4107, and 4115 terminals. It also supports the TK4106 terminal in a mode which reduces the amount of information which is put on the screen. The driver routine will interrogate the terminal before the first picture drawing instructions are sent. This series of terminals will respond with the model number which the driver routine remembers in issuing all subsequent drawing instructions.

9) VT240 This supports both the Digital Equipment Corporation (DEC) VT-240 and the VT-241 graphics terminals.

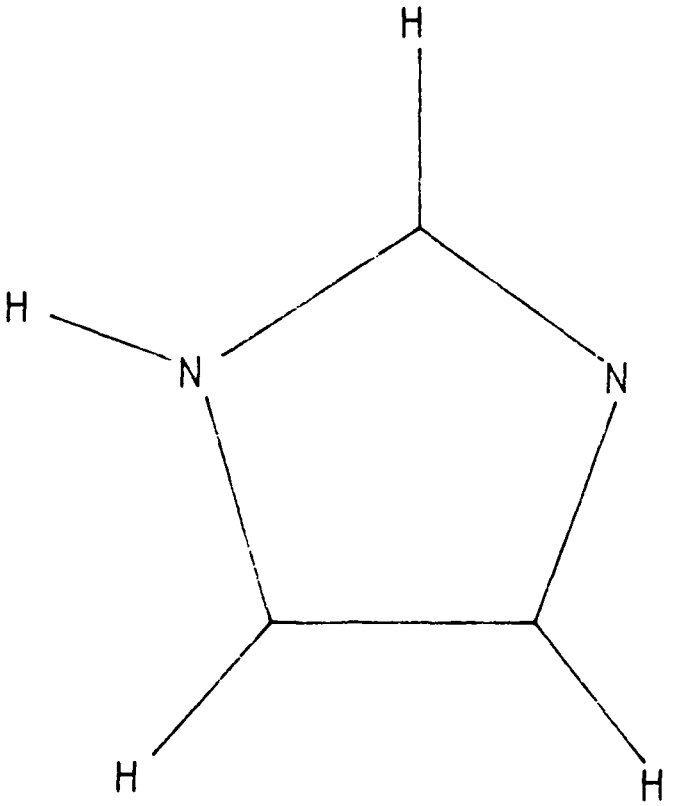

Figure 2. Imidazole shown with atomic symbols marking atom positions.

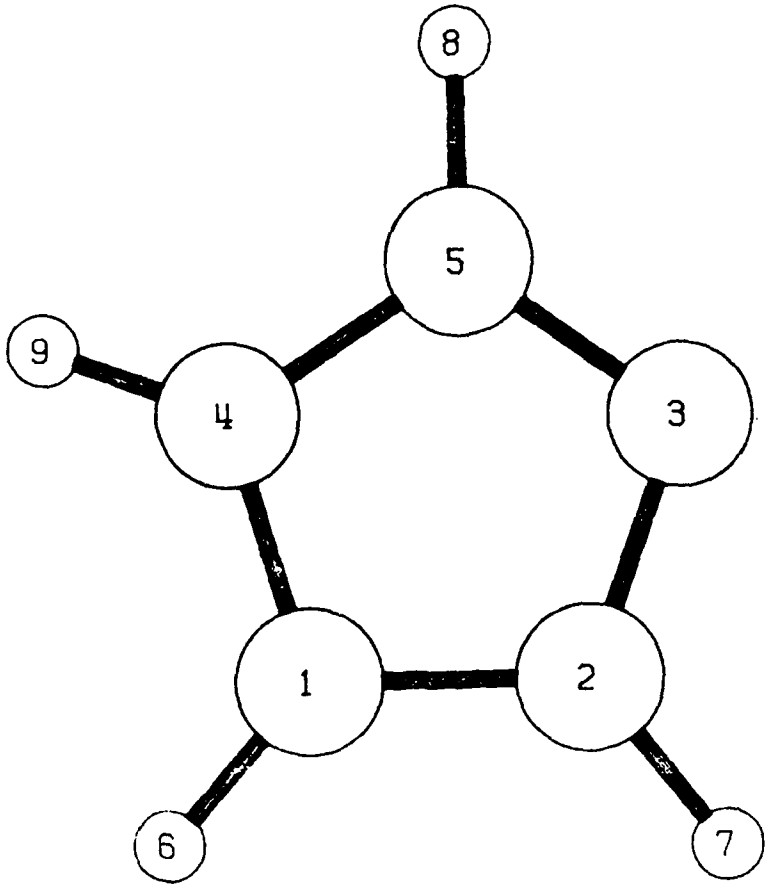

Figure 3. Imidazole shown in ORTEP representation.

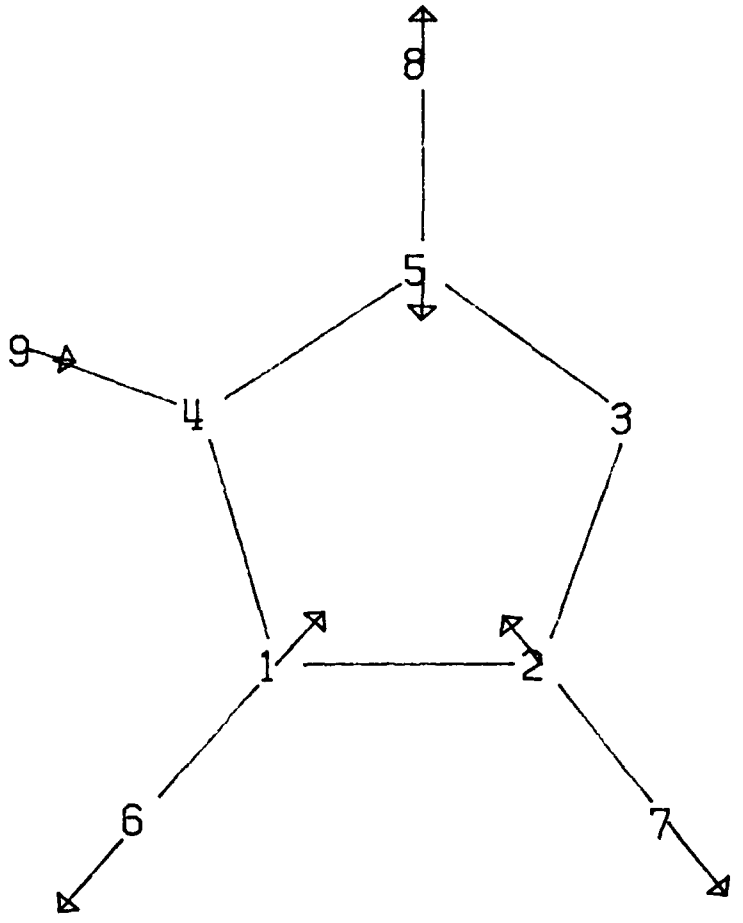

figure 4. Imidazole showing vibrational vectors.

CHAPTER 4

EDITING MOLECULES

4.1 INTRODUCTION

Perhaps one of the more frustrating aspects of molecular orbital calculations is designing an input geometry. Some of the more vexing problems are

A. Entering new geometry descriptions

B. Designing large ring systems

C. Eclipsing groups

D. Assembling polypeptides

E. Orientation of reacting species

F. Construction of big molecules

G. Combining two existing geometry files

Certainly, these are not overly difficult for small systems - but semi-empirical methods have matured to the point where drugs and polypeptides can be studied effectively.

DRAW has facilities which allow extensive editing of molecular geometries. The first, and most obvious, facility is the EDIT command. When you enter the EDIT routine, the picture is re-drawn (if needed) using STICK figures. This mode of display is chosen because it eliminates the problem of hidden line elimination and because, usually, lines can be erased individually rather than re-drawing the entire picture to change a few entries. The less obvious facilities include GIP and subcommands of ROTATE and MOVE.

Before we start discussing examples of EDITING geometries, one small feature of DRAW must be explained. The EDITING features expect that the user is making changes with the intent

of saving the resulting information for submission to a molecular orbital program. Therefore, after an EDITING change has been made DRAW will not allow you to QUIT without giving you a chance to OUTPUT the new geometry. If you do not wish to save the results of the editing you may simply repeat the QUIT command.

4.2 EDITING EXAMPLES

A. ENTERING NEW GEOMETRIES

Of course, you can use the text editor on your computer to create a new geometry file. Often users will copy an old file with a new name, edit the new file, and re-design the exiting description to create a new molecule. However, DRAW has some interactive features which can make the task easier. This is especially true if you use a variety of different computers. DRAW offers a uniform approach to creating data files.

To create a new data file with DRAW simply run DRAW the normal way. When DRAW asks for the name of the input file, enter the name you want to call your new file. When DRAW does not find the file, it will warn you but it will allow you to continue entering commands. Note that some of the DRAW commands will NOT function unless you have entered one or more atoms.

If you are using a graphic terminal which DRAW recognizes, you can tell DRAW which model you are using. DRAW will place the terminal in the graphic mode. But since you have not entered any atoms, no coordinates and no geometry will be seen.

Now enter the EDIT command. To begin entering new atoms, enter "+" and return. DRAW will prompt for the IC (internal coordinate) of atom 1. For the first atom enter the atomic symbol followed by nine (9) zeros:

```
C1  0  0  0  0  0  0  0  0  0
```

When you press return DRAW will erase the screen and draw the current geometry. Then DRAW will prompt for the IC of atom 2. Remember that atom 2 requires a distance from atom 1. When you enter the coordinates of atom 2 and press return, DRAW will again erase the screen and re-draw the geometry.

When you enter the coordinates for atom 3, DRAW will re-draw the geometry. However, for the fourth and subsequent atoms DRAW will not re-draw the geometry. Instead, subsequent atoms will be added to the display but their cartesian coordinates will not be listed. If any atom extends beyond the edge of the graphic area, the atom will not be displayed. (It will probably be show as a line on the edge of the screen.) If you wish to have the display re-drawn to include all atoms, stop entering new atoms by pressing return when DRAW asks for the next atom. DRAW will prompt for an EDIT subcommand. Enter PICTURE and DRAW will erase the screen and re-draw the geometry.

B. DESIGNING LARGE RING SYSTEMS

When designing large ring systems, closing the ring is a matter of accurate distances and angles. If the ring is not flat, your problems increase. DRAW's editing functions will allow you to rapidly construct large rings without accurate advanced knowledge of the necessary distances and angles. With interactive graphic display of the molecule and automatic bond selection, you will know immediately if the final atom actually closes the ring. If the ring does not close, you can go back and adjust each atom, as needed, until the ring does close.

Usually it is easier for a chemist to visualize and build an annular system using bond lengths, bond angles and "normal" dihedral angles. However, many geometry optimization routines (including those used in MOPAC) will encounter difficulties when using these relationships. In particular, as the optimization algorithm flexes the various angles, remote portions of the molecule may move through large distances. If this "cracking the whip" motion causes bonds between atoms to break and re-form, the optimization algorithm will probably fail.

After you construct the ring and achieve a reasonable starting geometry, DRAW can also help your geometry optimization routine. You can use the EDIT function to alter the connectivity of the atoms in the ring. However, you don't want the atoms to move when you change their definitions. By using CARTESIAN MODE in the EDIT command (see MODE subcommand) the atomic positions will be defined by their X, Y, and Z coordinates but the description will also include the connectivity required to re-form the internal coordinate description. Now you can alter any of the three component values without any of the atoms moving.

DRAW refers to the three as NA (distance reference atom of the internal coordinate description), NB (the angle reference), and NC (the dihedral reference).

The best method of describing geometries for MOPAC is to keep the normal definition of the bond length (i.e., don't change NA) but to define all angles and dihedrals with respect to either an atom (or dummy atom) outside the ring or with respect to the first two atoms of the ring. This way, when MOPAC flexes the various angles, the ring will not be greatly distorted. The EDIT command is all that is needed here. You have two ways of approaching this problem:

1. EDIT has a subcommand to ADD (see command +) new atoms to the end of a geometry description. Using this subcommand, you can actually build the ring system on the screen of your graphic terminal. As you enter the coordinate description of each atom, it will be drawn on the screen. If the last atom entered is not correctly placed you can DELETE it with the '-' and re-ADD it correctly. This process can be continued until you are satisfied with the result.

2. EDIT has a subcommand to modify the coordinates of any atom in the molecule. You simply type the number of the atom that you wish to alter. DRAW will display the current coordinate description which you can then alter with the proper subcommands. The effects of changed coordinates are posted immediately to the screen. In this way, you can alter an existing structure, atom by atom, to achieve the desired geometry.

C. ECLIPSING GROUPS There are, again, two methods available which can alter sections of the molecule. However, they are not equivalent. While one method may work for certain eclipsing problems, it may not work for all problems. You may have to experiment with the suggested methods to find the one which solves your problem.

1. The ROTATE command usually operates on the whole molecule. This is the default action. However, the ROTATE subcommand GROUP allows you to rotate any part or parts of the molecule. In fact, the parts do not have to be connected in any direct manner for this to be done. If, for example, you need to rotate a phenyl group to a different angle you would enter the ROTATE command followed by the

GROUP subcommand. At this time, DRAW simply notes that GROUP IS SET. Then you select the type of rotation and enter the other required information for the type of rotation desired. For the offending phenyl, you might wish to rotate it about the vector between the carbon atom connected to the rest of the molecule and the carbon atom directly across the ring with a rotation of 30 degrees. After the above information is entered, DRAW will then ask you to enter the information describing the GROUP which is to be rotated in the specified manner. After you enter the numbers of the atoms to be rotated (here they would be the numbers of the carbon atoms in the phenyl group along with the hydrogens attached to them), DRAW will rotate them and re-draw the new geometry.

2. If, however, all of the atoms in the group to be altered are related to each other via the coordinate description, you can use the EDIT command to achieve the same result in an easier manner. (To use EDIT the angles and dihedral angles for all atoms of the group must be related to the bridging atom of the ring.) After entering the EDIT routine, type the number of the phenyl carbon which is connected to the rest of the molecule, or the neighboring carbon atom which describes the dihedral (hence the tilt of the ring) and alter the value(s) of the coordinates. Again the geometry will be updated on the screen.

D. ASSEMBLING POLYPEPTIDES The obvious method of assembling a polypeptide, atom by atom, would be prohibitive. There are two alternatives using DRAW:

1. If the geometry is available via the BROOKHAVEN PROTEIN DATA BANK, DRAW can read the file structure with routine BPDBRD. This routine will allow you to select any parts of the geometry that you wish to use.

2. Alternatively, assuming that the individual units have been calculated previously and the geometries are available as input to DRAW, they can be used to construct the polypeptide. The normal method is:

   a) Start with one end of the final polymer

   b) Read in the geometry of the terminal unit

c) Use ROTATE to orientate it in an appropriate manner, e.g. place the atom involved in the linkage along the X-axis

d) Use EDIT to remove the hydrogen, if necessary

e) Use the GIP command to output a GIP file. See the chapter "GEOMETRY INTERCHANGE PROGRAM" for a more complete discussion of GIP.

f) Read in the geometry of the next peptide unit

g) ROTATE and MOVE it so the atom which will link with the atom of the previous unit(s) is at the origin and also along the X-axis

h) Use GIP to create an output file of this one, too

i) QUIT the DRAW program

j) Use your computer's text editor to combine both files and modify the internal coordinate references to properly reflect the desired connectivity, Be certain to remove the extra four text lines between the first geometry and the second geometry.

k) Run DRAW and draw the combined GIP file, if the units are not connected correctly, use either the text editor or the EDIT command to correct

l) Again ROTATE and MOVE to place the terminal atom along the X-axis, use GIP to output the combined file (this is not necessary if there were no changes made), and repeat the process for subsequent residues

m) Finally OUTPUT the total geometry of the finished polypeptide.

3. ORIENTATION OF REACTING SPECIES While this often seems to be a totally different problem, it can be handled in the same manner as for eclipsing groups which were discussed above.

4. BIG MOLECULES This is where DRAW really shines. You can start from a variety of sources of information:

1. Brookhaven Protein Data Bank
2. Other X-ray crystallographic sources
3. Previously optimized geometries from MOPAC, etc.
4. Psi/phi angles for peptides
5. Tables of bond lengths, angles, and dihedral angles
6. Your best guess

If your source is electronic (sources 1 through 3, above), DRAW can actually read the information. If you have psi/phi angle information for a peptide, you can also read most of the geometry with DRAW and simply provide the relation angle information. The MERGE subcommand in EDIT will read individual amino-acid files while you provide the missing six internal coordinates. (See the MERGE subcommand under EDIT.) For the other sources of data you will have to do a lot of typing, but DRAW's EDIT command can help you. For all of the methods of input, the interactive graphic display from DRAW will help you get the best trial geometry.

CHAPTER 5

GEOMETRY INTERCHANGE PROGRAM

The purpose of GIP is to provide the user with total control of the molecular geometry design process. Some geometry defining tasks or geometry re-defining tasks are too complex to perform with a generalized editing program. This is especially true within DRAW where the philosophy of action is to help the user by double checking the context of the geometry. If what you want to do is so complex that it requires more than two actions to complete, DRAW probably will not handle it. Use GIP for such tasks.

The GIP command produces an output file which you can edit after you exit DRAW. You should be able to use any normal text editor on your computer to do the editing.

The file contains four text lines followed by N+1 special cartesian geometry lines. The first text line is for internal identification by the DRAW program and should NOT be altered. The remaining three text lines contain the keywords, comments, and title line from the original input file and will be reproduced in any subsequent output file from the DRAW program. The remaining lines contain the atomic symbol, x, y, and z cartesian coordinates and the internal coordinate connectivity of the input file. These lines may be edited, by any suitable text editor, outside the DRAW program to alter the numbering, connectivity, or cartesian position of the atoms. Especially, you can alter the sequence of the atoms by changing the order of the lines in the file.

** NOTE: No special command is required to input a DRAW/GIP file, the DRAW program will recognize the special first line.

The utility of GIP can best be explained via an example. We can start with a typical internal coordinate description of, for example, benzene.

```
   POLAR SYMMETRY
   BENZENE

C     0.000000  0     0.000000  0     0.000000  0    0  0  0
C     1.406611  1     0.000000  0     0.000000  0    1  0  0
C     1.406611  0   120.000000  0     0.000000  0    2  1  0
C     1.406611  0   120.000000  0     0.000000  0    3  2  1
C     1.406611  0   120.000000  0     0.000000  0    4  3  2
C     1.406611  0   120.000000  0     0.000000  0    5  4  3
H     1.090244  1   120.000000  0   180.000000  0    1  6  5
H     1.090244  0   120.000000  0   180.000000  0    5  6  1
H     1.090244  0   120.000000  0   180.000000  0    2  1  6
H     1.090244  0   120.000000  0   180.000000  0    6  1  2
H     1.090244  0   120.000000  0   180.000000  0    3  2  1
H     1.090244  0   120.000000  0   180.000000  0    4  3  2
0     0.000000  0     0.000000  0     0.000000  0    0  0  0
2,    1,    3,
2,    1,    4,
2,    1,    5,
2,    1,    6,
7,    1,    8,
7,    1,    9,
7,    1,   10,
7,    1,   11,
7,    1,   12,
```

If the above internal coordinate description of benzene were converted to a GIP file by use of the GIP command, the resulting file would be:

```
GIP/DRAW DO NOT EDIT THIS LINE!  0.000000  0.000000  0.000000
   POLAR SYMMETRY
   BENZENE
     GEOMETRY INTERCHANGE EXAMPLE
C      0.000000 0     0.000000 0     0.000000 0    0     0     0
C      1.406611 1     0.000000 0     0.000000 0    1     0     0
C      2.109917 0     1.218161 0     0.000000 0    2     1     0
C      1.406611 0     2.436322 0     0.000000 0    3     2     1
C      0.000000 0     2.436322 0     0.000000 0    4     3     2
C     -0.703306 0     1.218161 0     0.000000 0    5     4     3
H     -0.545122 1    -0.944179 0     0.000000 0    1     6     5
H     -0.545122 0     3.380501 0     0.000000 0    5     6     1
H      1.951733 0    -0.944179 0     0.000000 0    2     1     6
H     -1.793550 0     1.218161 0     0.000000 0    6     1     2
H      3.200161 0     1.218161 0     0.000000 0    3     2     1
H      1.951733 0     3.380501 0     0.000000 0    4     3     2
0      0.000000 0     0.000000 0     0.000000 0    0     0     0
```

As the above example demonstrates, converting a file via GIP will lose some of the information in an internal coordinate file. Specifically, ymmetry and internal coordinate freedom information is removed. This information is removed because GIP

files are normally used in changing the connectivity of a molecular description.

The data in the GIP file consists of the atomic symbol, the cartesian coordinates, and the connectivity needed to reconstitute an internal coordinate file. After QUITTING DRAW, you can use a text editor to alter the description. Some possible changes include:

1. Inserting dummy atoms (or any other types of atoms)
2. Changing the internal coordinate connectivity
3. Altering the sequence of atoms
4. Altering the cartesian space position of atoms
5. Combining two separate geometry descriptions

Dummy atoms can be used in various ways. If you wanted to define benzene radially (i.e., as CH units radiating outward from a central point) a dummy atom could be entered as atom number one as:

```
XX    0.703306 0    1.218161 0    0.000000 0   0    0    0
```

Actually, we will add two dummy atoms so we can use them to define the distance and angle of all of the real atoms. The dihedral angles will specify the separation of the atoms. The internal coordinate connectivity of following atoms in the file must be altered to refer to the new atom and to reflect the new number of atoms in the description as:

```
 GIP/DRAW DO NOT EDIT THIS LINE!  0.000000  0.000000  0.000000
      POLAR SYMMETRY
      BENZENE
        GEOMETRY INTERCHANGE EXAMPLE
   XX      0.703306 0    1.218161 0    0.000000 0  0    0    0
   XX      0.703306 0    1.218161 0    2.000000 0  1    0    0
    C      0.000000 1    0.000000 0    0.000000 0  1    2    0
    C      1.406611 0    0.000000 0    0.000000 0  1    2    3
    C      2.109917 0    1.218161 0    0.000000 0  1    2    3
    C      1.406611 0    2.436322 0    0.000000 0  1    2    3
    C      0.000000 0    2.436322 0    0.000000 0  1    2    3
    C     -0.703306 0    1.218161 0    0.000000 0  1    2    3
    H     -0.545122 1   -0.944179 0    0.000000 0  1    2    3
    H     -0.545122 0    3.380501 0    0.000000 0  1    2    3
    H      1.951733 0   -0.944179 0    0.000000 0  1    2    3
    H     -1.793550 0    1.218161 0    0.000000 0  1    2    3
    H      3.200161 0    1.218161 0    0.000000 0  1    2    3
    H      1.951733 0    3.380501 0    0.000000 0  1    2    3
    0      0.000000 0    0.000000 0    0.000000 0  0    0    0
```

After editing the above saved file, save the modified form and exit the editor. Run DRAW and specify the new file for input. DRAW will draw the new picture (which should look exactly like the starting picture). Then you OUTPUT a new file from DRAW. The resulting output file will look like:

```
      POLAR SYMMETRY
      BENZENE
        GEOMETRY INTERCHANGE EXAMPLE
 XX     0.000000   0    0.000000   0    0.000000   0  0    0    0
 XX     2.000000   1    0.000000   0    0.000000   0  1    0    0
 C      1.406611   1   90.000000   1    0.000000   0  1    2    0
 C      1.406611   1   90.000000   1  -59.999994   1  1    2    3
 C      1.406611   1   90.000000   1 -120.000015   1  1    2    3
 C      1.406611   1   90.000000   1  179.999965   1  1    2    3
 C      1.406611   1   90.000000   1  119.999970   1  1    2    3
 C      1.406612   1   90.000000   1   59.999985   1  1    2    3
 H      2.496855   1   90.000000   1    0.000000   1  1    2    3
 H      2.496855   1   90.000000   1  119.999977   1  1    2    3
 H      2.496855   1   90.000000   1  -60.000003   1  1    2    3
 H      2.496856   1   90.000000   1   59.999985   1  1    2    3
 H      2.496855   1   90.000000   1 -120.000015   1  1    2    3
 H      2.496855   1   90.000000   1  179.999974   1  1    2    3
 0      0          0    0          0    0          0  0    0    0
```

Rounding errors within DRAW cause the non-exact dihedral angles. Notice that the keyword "SYMMETRY" is still there but that there are no symmetry specifications at the end of the file - many of the original ones are now meaningless. (See the MOPAC manual for a description of the SYMMETRY keyword.) Also, all of the internal coordinates are now marked for optimization - even the dummy atoms. You will have to use the text editor again to

fix things up the way you want them. This may seem like a lot of effort for a simple molecule like benzene, but for a large molecule, the effort is more reasonable.

CHAPTER 6

DRAW FILES

6.1 INTRODUCTION

The DRAW program accepts input from a variety of files and, in turn, can create a number of output file types. Most types are related directly to the two programs MOPAC and DENSITY. For input files, the type of file is recognized by the subroutine GPRDR, the general purpose reader, by analyzing the first ten lines of the file. Thus, the input file may be called by any name. On the other hand, the default name of an output file is related to the name of the input file and the DRAW command which produced the output.

The use of extensions on a root file name, eg. "ETHYLENE.DAT" or "NEOMYCIN.ARC" is rather computer, or, more properly, operating system, dependent. Since MOPAC, DENSITY, and DRAW were developed on VAX computers, the syntax of file names were chosen to conform to VAX standards. However, the code which recognizes and creates file names is easy to follow and is located in the main routine of DRAW. Input and output files are opened (and closed when necessary) by FORTRAN-77 commands, thus removing the need for complicated command procedures external to the DRAW program.

6.2 INPUT FILES

Input file types which DRAW recognizes are:

A. MOPAC file types

1. MOPAC INPUT FILE (VAX file extension: DAT) DRAW stores the first three lines of text from this type of file and can output them as: keywords, comment, and title in subsequent files. In addition, DRAW processes the internal coordinate description which

it can use in all DRAW commands. The optimization flag integers from the coordinate description are also stored but some output requests destroy them. DRAW does not store reaction path points.

2. MOPAC OUTPUT FILE (VAX extension: OUT) DRAW can handle most parts of MOPAC output files:

   a) internal coordinate description

   b) heat of formation

   c) normal component of the geometry gradient

   d) charge

   e) electronic eigenfunctions

   f) atomic charges

   g) normal modes of vibration

3. MOPAC ARCHIVE FILE (VAX extension: ARC) DRAW processes all information common between archive files and output files.

B. DENSITY file (VAX extension: TEC) This file is a cross-sectional representation of the electronic density picture produced by the DENSITY program. DRAW does no real processing on this information; rather it provides a convenient means of displaying DENSITY output on a graphic terminal.

C. DRW FILE (VAX extension: DRW) This is a special category of files. Many of them have been supplied with your distribution tape of DRAW. This is an internal coordinate file formatted exactly as a DATA file. The unique extension is intended to keep them separate from MOPAC type files. The DRW files distributed with DRAW have been optimized with PRECISE and via the AM1 Hamiltonian. You can add more DRW files to your collection.

D. HELP FILE (VAX extension: HLP) This file, DRAW.HLP, is distributed with the DRAW program. The user is not encouraged to modify this file. DRAW opens this file to provide assistance in response to the HELP command.

E. GEOMETRY INTERCHANGE PROGRAM FILE (VAX extension: GIP) This type of file is both an input and an output file for DRAW. It is not intended to be used as input or output with any other program. For more information, see the chapter on GIP.

F. BROOKHAVEN PROTEIN DATA BANK FILE (VAX extension: BPD) DRAW accepts data from an unpacked file from Brookhaven Protein Data Bank distribution tapes. The data on the distribution tape is packed with more than one record per tape block. DRAW does not have code to unpack this blocking. The user has two possible actions:

1. Use operating system functions to assign the magnetic tape in such a manner to automatically unpack the data before DRAW reads each line.

2. Use an external program to unpack the files from the tape to produce a file which has only one record per block. Then invoke DRAW to read the unpacked file.

6.3 OUTPUT FILES

Output files which DRAW can create are:

A MOPAC DATA FILE (VAX extension: DAT) This is the principal result of the editing capability of DRAW. The OUTPUT command creates a file which contains the current geometry description and is correctly formatted for MOPAC. If a previous data, archive, gip, or output file was used to start the editing session, the keywords, comment, and title lines will contain the same text as in the starting file.

B DRAW GRAPHICS OUTPUT (VAX extension: PLT) The PLOT command produces a file which contains the commands which will create a copy of the molecular picture on a selected hardcopy output device. DRAW supports both bit-mapped and plotting types of devices. Check the list under the subcommand PLOT which is listed under the command DISPLAY.

C MOLECULAR MECHANICS (VAX extension: MMI) The DRAW command MMI will convert the current geometry to a file formatted for input to Molecular Mechanics II (QCPE 423). Note that DRAW cannot read Molecular Mechanics

output files.

D GEOMETRY INTERCHANGE PROGRAM (VAX extension: GIP) This type of file is both an input and an output file for DRAW. It is not intended to be used as input or output with any other program. For more information, see the chapter on GIP.

CHAPTER 7

TERMINAL SUPPORT

DRAW attempts to support all terminals in an identical manner. For this reason, you will find that some more exotic terminal features are not exercised by DRAW. Some of the features often found on terminals but not used by DRAW include:

1. manual input of graphic positioning (eg. mouse, cross-hairs)

2. internal, graphic character sets

3. graphic area filling or shading

4. automatic terminal identification

5. internal 3-D representation

6. internal hidden line elimination

I have not found a method of supporting these features on only some terminals while continuing support of older terminals. I have added color support of terminals for the Tektronix 41XX series and the Terak 8600 terminals. For other terminal capabilities, you should experiment a little. For example, we have found that DRAW functions in a neat manner with our Tektronix 4107 terminal. This terminal has hardware zoom and pan. While zoomed-in on a specific portion of the molecule, we have found that EDIT functions are displayed in proper perspective in the display area. This ability was not expected (without intensely reading the terminal manuals) and we were pleasantly surprised when it worked.

Because only common functions of terminals are used, anyone can add a new type of terminal. Different models of terminals are identified within DRAW by the integer variable, TTYPE. Quite a few different types of terminals may be supported.

On a DEC VAX computer using the VMS operating system, a special system subroutine, "LIB$SCREEN_INFO", is called to identify the type of terminal. The resulting value from this call is translated to a terminal number within DRAW at the begining of the module DRAWII. For support of other types of terminals this code may be modified along with the block of code, also in DRAW2, which handles the TERMINAL command, and the IF-THEN-ELSEIF code in module PLOT which calls the appropriate terminal driver routines. For other computers or operating systems, the first block of code in DRAW2 (the block associated with LIB$SCREEN_INFO) may be removed and the integer variable TTYPE may be assigned to the specific value you select. Of course, the user may use the TERMINAL command to select the proper terminal type at any time while running the program.

If you need to add support for other terminals, their driver routines must meet the following protocol:

1. The terminal driver is called by subroutine PLOT. The calling line will contain three variables:

   A. X - A real (i.e. floating point) variable which contains the X-COORDINATE for the current directive. (This will range from 0.0 to 1.0.)

   B. Y - A real variable which contains the Y-COORDINATE for the current directive. (This will range from 0.0 to 1.0.)

   C. IND - A integer variable which contains the code value for the current directive.

2. The permitted values of IND have the following meanings:

   (0) Clear al graphic structures (segments, etc.) prior to exiting from DRAW.

   (1) This is the time to perform any one time only initialization of the terminal. E.g., setting the number of coordinate lines in the display, setting the text scroll area, and setting the number of colors available.

   (2) Move the "graphic cursor" or position to the specified X and Y value. no line is drawn.

   (3) Draw a line in the current color or style from the last point (referenced by IND=2 or IND=3) to the new point. Make the new point the last point referenced for any subsequent IND=3 directives.

(4) Draw a dark line which erases a previously drawn line by drawing back over in the background color.

(5) Draw a bright (visible) line. This is the starting mode for drawing.

(6) Initialize the terminal for drawing the next picture.

(7) Not used.

(8) Temporary release from graphics. This directive is used to communicate with the user in a manner (or an area of the screen) which does not interfere with the current picture. This directive, and IND=9, may be called at any time during or after drawing a picture.

(9) Return to graphics. This directive is used to communicate with the user in a manner (or an area of the screen) which does not interfere with the current picture. This directive, and IND=8, may be called at any time during or after drawing a picture.

(10) Done drawing the current picture - but do not erase the picture.

(99) Select next color for visible lines. The value of the color is contained in the variable X.

Use of other values of IND should be avoided to ensure compatability with future versions of DRAW.

For Tektronix 4010, 4014, 4105, 4107, 4115 (and related) terminals your computer must pass the FORMFEED character (character number 10) through unaltered. If your computer does not, the screen will not get erased when it contains graphics. You may have to contact your computer center to get around this.

CHAPTER 8

INSTALLING DRAW

8.1 FIRST TIME INSTALLATION

DRAW is distributed on a magnetic tape as a set of FORTRAN-77 files, along with ancillary documents such as help files and a line printer version of this manual. The format of the tape is that of the VAX-11/780 computer unless other arrangements have been made. (In general: the tape starts with an ANSI tape label. The label name is DRAW. The tape is not blocked. Each record is variable length. There are multiple files on the tape.) The following instructions apply only to users with VAX computers; users with other machines should use the following instructions only as a guide to getting DRAW up and running.

1. Put the magnetic tape on the tape drive, making sure it is write protected. This is always a good idea when working with the original magnetic copy of any program. You write protect a magnetic tape by removing the plastic ring from the groove around the spindle hole on the back side of the tape reel.

2. Allocate the tape drive with a command such as $ALLOCATE MTA0:

3. Go into an empty directory which is to hold DRAW

4. Mount the magnetic tape with the command $MOUNT MTA0: DRAW

5. Copy all the files from the tape with the command

   $COPY MTA0:*.* */LOG

   If this command does not work, try

```
$COPY/LOG MTA0:*.* *
```

A useful operation after this would be to make a listing (or hard copy) of the contents of the directory. You should now have the following sets of files in the directory:

1. A set of FORTRAN-77 files, see Appendix C.
2. The command file COMPILE.COM and the auxiliary file DRAW.OPT.
3. A help file called DRAW.HLP, see Chapter 3.
4. A text file of this document, DRAW.MAN.
5. A set of files which end in ".DRW", see Appendix D.

STRUCTURE OF COMPILE COMMAND FILE

The parameter file SIZES.CMN should be read and, if necessary, modified before COMPILE is run. COMPILE should be run only once. The COMPILE command reads the file "DRAW.OPT" to know which files must be compiled to produce DRAW.

All the FORTRAN files are then compiled, using the array sizes given in SIZES.CMN. These should be modified before COMPILE is run. If, for whatever reason, SIZES.CMN needs to be changed, then COMPILE should be re-run, as modules compiled with different SIZES.CMN will be incompatible.

The two parameters within SIZES.CMN that the you can modify are MAXLIT and MAXHEV. MAXLIT is assigned a value equal to the largest number of hydrogen atoms that a DRAW job is expected to run, MAXHEV is assigned the corresponding number of heavy (non-hydrogen) atoms.

When everything is successfully compiled the command procedure will ask if you wish to create DRAW.EXE. The object files will then be linked into an executable image called DRAW.EXE. Once the image exists, there is no reason to keep the object files, and if space is at a premium these can be deleted at this time.

Next the command procedure will ask if you wish to create DRAW.HLB. This is not necessary but does provide a convenient source of help without the necessity of executing DRAW. If you create DRAW.HLB, the procedure will search for the next

available help library name. Write this name on a piece of paper -- or here in the manual for later use.

Name of HELP LIBRARY _____

A recommended sequence of operations to get DRAW up and running would be:

(1) Modify the file SIZES.CMN; the default sizes are 250 heavy atoms and 250 light atoms.

(2) Edit the login command file to insert the following lines:

```
$ASSIGN DBA0:[DRAW]           DRAWDIRECTORY      (Note 1)
$ASSIGN DBA0:[DRAW]DRAW       HLP$LIBRARY_n      (Note 2)
$ASSIGN DBA0:[DRAW]DRAW.HLP   DRAWHELP           (Note 3)
$DRAW :== RUN DRAWDIRECTORY:DRAW                 (Note 4)
          (look at LOGIN.COM at this point.)
```

Note 1: Substitute the actual name of the directory which will hold DRAW if the name is not to be [DRAW]. If you cannot identify the directory, remove all references to DRAWDIRECTORY from the COMMAND files.

Note 2: This allows the VAX VMS HELP facility access the DRAW help library. If HLP$LIBRARY is already assigned, then use the first empty library, HLP$LIBRARY_n. The assignment may have to be modified.
(Consult someone who understands this!).

Note 3: This assignment is the means by which DRAW will access help information while executing. On a non-VAX computer the name of the help file may have to be changed in routine HELP.

Note 4: This assigns the word DRAW to run the executable file DRAW.EXE.

(3) Execute the modified LOGIN command so that the new commands are effective.

(4) Run COMPILE.COM. This takes about 30 minutes to execute.

(5) Enter the command $DRAW.
You will receive the identification message from DRAW which will ask for the input file to use.
The reply should be the actual data-file name. For example, "ETHYLENE", the file is assumed to end in .ARC, e.g. ETHYLENE.ARC.

8.2 UPDATING DRAW

Due to the number of changes I have made in DRAW, the best way to update DRAW is to start from the begining. First rename the old DRAW or copy it to a safe area. This will protect it incase you are unable to install the new version. Install the new DRAW in a new area of your computer before you delete all of the old DRAW. Since you already have made the definitions for the help library and DRAW command, you can skip steps 2 and 3, above. You especially want to ignore the designation for the help library if you already have that defined.

8.3 USING SOMEONE ELSE'S DRAW

If someone else has already gone to the trouble to install DRAW, you may be in luck. On a VAX computer you will need EXECUTE permission in each directory level to access the ENTIRE directory structure to the executable file, DRAW.EXE. The owner is the person to contact because he or she will have to grant you the necessary access. You will also need permissions to access the help library. You will need to insert the command lines shown in step 2, above, to easily use the other person's copy. Proceed with caution: if your files reside on a different disk drive from DRAW your commands will have to specify the correct disk drive name.

For two independent users, it may be worth asking the manager of the computer to establish DRAW and its help library as a common use program. This may save you the disk space needed to hold all of DRAW. Also the computer manager can grant special permissions to the program which can increase the available memory to draw large molecules. Check with the manager for this.

8.4 OTHER COMPUTERS

We have not tried DRAW on other computers. Despite my efforts to write in standard FORTRAN-77, I have never had the occasion to move DRAW to any computers other than DEC VAX's. We have networks which connect our other computers to VAX computers. The first thing to look for is that DRAW uses ALL of the FORTRAN-77 language standard. If your computer supports only the sub-set of FORTRAN you will probably have difficulty moving DRAW. Often the greatest deficiency lies in character string manipulation. String concatenation and sub-string extraction are used in all parts of DRAW. Refer to the chapter on DEBUGGING DRAW for the few areas of non-standard FORTRAN which may not be

supported on your [illegible] a knowledgable person how to create [illegible] cause DRAW to execute and how to [illegible] to allow DRAW to access the help library.

8.5 TERMINAL PARAMETERS

When you install DRAW on your (or someone else's) computer you may have to alter [illegible] the settings on the computer for proper control of the [illegible] are some things to look for. This [illegible] covers some of the problems [illegible].

If you are [illegible] terminal, your computer must be able to [illegible]. On some computers this is considered [illegible] occasionally intercepted by [illegible] formfeed character is not sent, the [illegible] simple problem is the tab character [illegible] of a graphics address. You may [illegible] your computer replaces the [illegible] character. The 4010 needs some other [illegible] that had problems with them.

On the Tektronix [illegible] terminals the formfeed character [illegible] screen. If DRAW fails to clear the [illegible] the formfeed character. The [illegible] character. This does not present serious [illegible] letters.

The Tektronix [illegible] one special character. All of the [illegible] text characters. However one of the characters [illegible] a command. In DRAW, the Tektronix [illegible] the command character is the exclamation [illegible] be altered in either your terminal or [illegible] of DRAW. If you alter the copy of DRAW, be sure [illegible] character which your computer can send.

In general, DRAW [illegible] of characters to create the display. [illegible] which do not require line carraige return [illegible] commands, DRAW does not send any. [illegible] which automatically sends carriage return [illegible] characters you will have to change [illegible]. On a DEC VAX this is altered by removing "[illegible]" from the settings.

CHAPTER 9

DEBUGGING DRAW

Before you go any further let me state that DRAW has been extensively tested - and not simply tested, but used routinely by a lot of chemists. You should not have to fix anything. But you may want to modify some default functions or transport the code to another computer. So let's look at four aspects of debugging:

1. Size of molecule DRAW can handle
2. Default parameters
3. Non-standard FORTRAN
4. In-place debugging logic

These four areas should cover routine situations when you would have to go into the code.

SIZE OF DRAW This is set via two parameters in SIZES.CMN, MAXLIT (the number of hydrogen atoms) and MAXHEV (the number of non-hydrogen atoms.) Chapter 8 describes this along with the installation of the program and its associated files.

DEFAULT PARAMETERS All of DRAW's functions are selected by variables. All of the variables are initialized in the mainline (i.e., the non-subroutine) section of DRAW which is named DRAW2. You may wish to alter one or more of the following features:

1. Default input file extension. This is carried in the variable EXTIN and is currently initialized to ".ARC".
2. Default output file extension. The variable EXTOUT is initialized to ".DAT".
3. Default off-line plotting file. This is stored in the variable EXTPLT and currently is equal to ".PLT".

4. Terminal type. The variable is ITYPE and is initialized to 0 to indicate a NON-GRAPHIC terminal.

5. Style of drawing. This option is held in the variable ISTYPE and is currently initialized to 0 for STICK drawings.

6. Default off-line plotting device. The type of off-line device is identified via the contents of the variable JHDEV which is currently set to 2 for an EPSON FX-80 matrix printer.

7. Style of labelling for atom positions. This variable, LATYPE is set to 1 for atom numbers.

8. Masking and allowing atoms. Whether an atom is drawn in the picture is controlled by two arrays (actually vectors because they are 1-dimensional). The first vector is IREM which is 200 integers long. Each location corresponds to an atomic (not atom) number. If the entry is 0 (zero) that type of atom is permitted. Hence, to allow hydrogens in the picture a 0 should be placed in the first location of IREM. The additional positions in IREM (those beyond element 103) are for special symbols such as XX for dummy atoms. Currently, dummy atoms are not allowed by default but all others are allowed. If you wish to prevent another atom from being drawn, you can insert a line of code in DRAW2. For example, IREM(43) = 1 will prevent Technetium from being drawn. If the undesirable atom type is a pseudo-element (above 103) then count the entries in ATSYMB which is also in DRAW2. The other vector is IMASK which has a location for every possible atom in the picture. Thus, the length of this vector is controlled by the parameters in the SIZES.CMN file. A non-zero entry in this vector prevents a specific atom from being drawn. For example, if you place a 1 (one) in the fifth location of IMASK, then the fifth atom of the molecule will not be drawn in the picture. Currently all atoms are allowed in the drawing.

NON-STANDARD FORTRAN - I have removed nearly every line of code which was not standard FORTRAN 77 from DRAW. However, for convenience of programming and user interaction there are THREE areas where non-standard code was intentionally left in:

1. INCLUDE - Nearly every source module includes a file named "SIZES.CMN". This file simply defines PARAMETERS (in the FORTRAN sense) which define the size of arrays in DRAW and often sets the limits of loops. The variables used are exactly the same as used in MOPAC so

DRAW should be able to read, write, or draw any MOPAC file that you can create if you use the same size defining file for both. Most compilers have some form of an "INCLUDE" command. You may have to alter the syntax of the current line but that should be no problem. If you compiler does not have any thing like the "INCLUDE" command, you should use the text editor to manually include the SIZES.CMN file everywhere it is needed. Be sure to remove the original INCLUDE command from the file. For your future reference you may wish to put a "C" in the first character position of the INCLUDE line rather than remove the line. This may seem a tedious job, but it is guaranteed to work. Before you do the manual fix, check with your computer center to insure your compiler dosen't have a similarly acting command with a different name or a separate "FIX UP" program.

2. OPEN - DRAW opens the input file in the subroutine GPRDR. The FORTRAN OPEN statement as implemented on a VAX computer allows an optional argument to allow the file access to be specified. In DRAW the file is opened with the access READ and SHARE. Thus, other programs (eg. MOPAC) can read the file as DRAW is reading it. If your computer does not support such access specifiers they can be removed. The result will be only a minor inconvenience.

3. UPROMP - Whenever DRAW needs to ask the user a question, the text is printed on the terminal via the subroutine UPROMP. My preference when conducting a dialog with a computer is to respond to questions on the same line as the question is written. In VAX FORTRAN, the automatic carriage return can be suppressed by a special FORMAT symbol, "$". You may have to do some searching to determine how your computer handles carriage returns. In MICROSOFT FORTRAN, the same feature requires "\". If your computer's FORTRAN does not support this type of control alter the FORMAT statement in subroutine UPROMP to remove the "$" symbol. The only effect will be more lines required to interact with the program.

IN-PLACE DEBUGGING LOGIC - DRAW has one command which is NOT documented in previous chapters. The DEBUG command activates selective debugging code throughout DRAW. If you type DEBUG (followed by a return) DRAW displays:

```
DEBUG:    L  N  O  P  I
          F  F  F  F  F  F
Draw: DEBUG>
```

The display indicates that all debugging logicals are FALSE. At

this point, in response to the prompt, you may turn on any of the areas of debug code. The commands (and sections) are:

1. D - General debug code in mainline of DRAW. This is the one with no letter above it.

2. L - Turns on debug code in LINE (or STICK) code.

3. N - Turns on debug code in NAMODI.

4. O - Activates debug code in ORTEP package.

5. P - Turns on debug code in general PLOTTING code.

6. I - Debug code in INPUT file logic.

7. - No entry exits DEBUG selection and resumes normal DRAW activity. If you selected any debug sections, they are now active.

These subcommands are toggles; the same letter will turn off a selected section.

If you select ORTEP and INPUT debugging (two separate commands), the display would look like:

```
DEBUG:    L  N  O  P  I
          F  F  F  T  F  T
Draw: DEBUG>
```

Use caution: some of these debug codes will generate copious amounts of text!

APPENDIX A

COMMAND REFERENCE PAGE

This appendix is a one page listing of all DRAW commands and sub-commands. The intention is to allow you to make copies to leave at all terminals you and your co-workers use. It will help you remember the available commands. Once you know the name of a command, you can either look it up in the manual or use the on-line help facility.

The commands are listed on the next page.

```
BELL

COMMAND

DISPLAY
  +/-##
  +/-S
  BONDS
    MATRIX
    RADII
    USER
  COORDINATES
  HELP
  LABELS
    BOTH
    MASK
    SYMBOLS
    USER
  MAP (COLOR)
  MO
  ORTEP
  PLOT
  QUIT
  SCALE
  TITLE
  VIBRATION
  ZOOM
    MANUAL
    OPTIMIZED
    SURFACE

EDIT
  +
  -[##]
  ##
    ANGLE
    BOND
    DIHEDRAL
    IA
    IB
    ID
    NA
    NB
    NC
    X
    Y
    Z
  DUMMY
  EDIT
  INFORMATION
  MERGE
  PICTURE
  UPDATE

HELP

GIP <FILE> [##]

INFORMATION
  ##[,##[,##[,##]]]
  BOND ORDER
  COUNT
  DIMENSION
  FILE
  HELP
  INFORMATION
  NEAREST
  QUIT
  RADIUS ## [R] [S]
  SYMMETRY
  TERMINAL
  VALENCE

LAST

MOVE
  CARTESIAN
  INTERNAL

NEXT
  [+]##
  RESET

OUTPUT <FILE>

PLOT <FILE> [SCALE]

QUIT

REFLECT
  XY/YZ/XZ
  INVERT

RESET

ROTATE
  CARTESIAN
  EULERIAN
  GROUP
  HELP
  PAIR
  NOGROUP
  QUIT

SYMMETRY

TERMINAL
```

APPENDIX B

SUBROUTINES

B.1 ROUTINES IN ALPHABETICAL ORDER

ARCRD	EIGEN	LAP800	NACLDI	PTDOT	TEKSTR
ATOM	EPSON	LAPAB	NACSCA	PTIGER	TERAK
AXEQB	ERPNT	LAPCON	NALIDI	PTLABL	TK4010
AXES	F1000	LAPDRW	NALILI	PTLINE	TK4025
AXIS	F200	LARROW	NAMODI	PTOPEN	TK4105
BANGLE	F400	LARROW	NAPARM	PTOPEN	TMM
BITDOT	F500	LATOM	NAPLOT	PTOUT	TOTROT
BITLBL	F600	LBOND	NAPOCA	PTOUT	UNIT
BITLIN	F700	LCLEAN	NAPRIN	QUIT	UPROMP
BMCLR	F800	LDRAW	NARACA	RADIAL	VECRED
BOND	F900	LLINE	NASIM	RCART	VM
BPDBRD	GEORD	LPLOT	NATTHE	READER	VTLINE
C4010	GETGEO	LSIM	NAXYIN	RESCOL	VXV
CLP240	GETIC	MATIN	NAXYTH	RETCLP	WRITE
CONTUR	GETSYM	MERGE	NORM	RETROG	XYZ
CORRD	GIGI	MINMAX	NUCHAR	RETSTR	XYZMND
DANG	GIPOUT	MM	NUMBUR	REULR	XYZMOV
DEBUGR	GIPRD	MMIOUT	OPLOT	ROTATE	
DEC240	GMETRY	MNDMOV	OSIM	ROTSUM	
DECSTR	GPRDR	MNDOUT	OUTPLT	RPAIR	
DIFV	GROUP	MOVE	PAXES	SCRIBE	
DIHED	GTEXT	MOVES	PICTUR	SEARC	
DISPLY	HALPLT	MPI99	PLOT	SETLAB	
DORTEP	HELP	MV	PLOTS	SETTRM	
DRAW	HQRII	NAAPSE	PLTXY	SETVEC	
DRELIM	INFO	NAARC	PRIME	SIMBOL	
EDIT	DRCRD	NACICI	PROJ	SPARE	
EDITAD	LA50	NACIDI	PTCLN	ST4010	
EDITCH	LAP500	NACILI	PTCLN	STOR	
EDITIN	LAP700	NACIRC	PTCLR	TEKCRD	

B.2 SPECIAL INPUT/OUTPUT ROUTINES

CONTOUR

B.3 GENERAL CONTROL ROUTINES

AXIS	BANGLE	DANG	DIHED	DISPLAY	DRAW2
EDIT	GENCOR	GETIC	GIPOUT	GROUPS	HELP
HQRII	INFO	MINMAX	MMIOUT	MNDMOV	MNDOUT
MOVE	OUTPLT	PICTURE	PLOT	QUIT	RCART
REULR	ROTATE	ROTSUM	RPAIR	SETTRM	TOTROT
XYZMND	XYZMOV				

B.4 STICK DRAWING ROUTINES

LARROW	LATOM	LBOND	LDRAW

B.5 NAMODI DISPLAY ROUTINES

NAAPSE	NAARC	NACICI	NACIDI	NACILI	NACIRC
NACLDI	NACSCA	NALIDI	NALILI	NAMODI	NAPARM
NAPOCA	NAPRIN	NARACA	NATTHE	NAXYIN	NAXYTH

B.6 ORTEP DISPLAY ROUTINES

ATOM	AXEQB	AXES	BOND	DIFV	DRAW
EIGEN	ERPNT	F1000	F200	F400	F500
F600	F700	F800	F900	LAP500	LAP700
LAP800	LAPAB	LAPCON	LAPDRW	MERGE	MM
MOVES	MV	MYORTEP	MYPRELIM	NORM	NUMBUR
PAXES	PLOTS	PLTXY	PRIME	PROJ	RADIAL

RDBYTE	SCRIBE	SEARC	SIMBOL	SPARE	STOR
TABLE	TMM	UNIT	VM	VMV	VV
VXV	XYZ				

B.7 BITMAP GRAPHIC ROUTINES

BITDOT	BITLIN	BMCLR	PTCLN	PTCLR
PTLINE	PTOPEN	PTOUT		

B.8 GENERAL INPUT ROUTINES

ARCRD	BPDBRD	CLEAN	CORRD	ELEMNT	ELEMNT
GEORD	GETSYM	GIPRD	GMETRY	LCLEAN	NUCHAR
READA	UPCASE	UPROMP	WRITE		

B.9 TERMINAL CONTROL ROUTINES

DTERAK	EPSON	HALPLT	LA50	MPI99	ST4010
TEKCRD	TEKSTR	TERAK	TIGER	TK4010	TK4025
TK4105	VT240				

B.10 COMMON DATA AREAS

COMMON: ORNL

ATOM	BOND	DRAW	EIGEN	ERPNT
F200	F400	F500	F600	F700
F800	F900	LAP500	LAP700	LAP800
LAPAB	LAPDRW	MERGE	DORTEP	DRELIM
NORM	PAXES	PLTXY	PRIME	RADIAL
SEARC	SPARE	STOR	UNIT	XYZ

COMMON: ALLROT

DRAWII	ROTSUM	TOTROT

COMMON: ASCIIC

DRAWII	TK4105	NAPRIN	CONTUR

COMMON: ATMASS

DRAWII	AXIS

COMMON: ATOMS

DRAWII	EDIT	GIPOUT	INFO	MINMAX
MMIOUT	MNDMOV	MNDOUT	MOVE	ROTATE
TOTROT	XYZMND	XYZMOV	LATOM	LBOND
LDRAW	NAAPSE	NACIDI	NACIRC	NACLDI
NALIDI	NAMODI	NAPRIN	DORTEP	DRELIM

COMMON: ATSYMB

DRAWII	DISPLY	EDIT	GETIC	GIPOUT
INFO	MMIOUT	MNDOUT	LATOM	NACIRC
NAPRIN	DRELIM			

COMMON: COMM

DRAWII	DISPLY	INFO	MOVE	ROTATE

COMMON: DEBCOM

DRAWII	EDIT	GENCOR	GETIC	GIPOUT
HELP	INFO	MMIOUT	MOVE	PLOT
RCART	REULR	ROTSUM	RPAIR	TERAK
TK4105	TOTROT	XYZMOV	LATOM	LBOND
LDRAW	NAAPSE	NACIRC	NAMODI	BOND
F800	LAP500	DORTEP	DRELIM	SEARC
SIMBOL	GIPRD	LCLEAN	WRITE	VTLINE

COMMON: DENSTY

DISPLY

COMMON: DEVICE

DRAWII NAPRIN

COMMON: DISPLY

DRAWII	DISPLY	EDIT	HALPLT	INFO
MINMAX	MMIOUT	PICTUR	PLOT	OUTPLT
TK4025	TERAK	TK4105	PTIGER	LATOM
LBOND	LDRAW	NAAPSE	NACIDI	NACIRC
NACLDI	NALIDI	NAPRIN	DORTEP	DRELIM
WRITE	CONTUR			

COMMON: EDIT

DRAWII	DISPLY	EDIT	MOVE	RCART
REULR	ROTATE	RPAIR		

COMMON: FINFO

INFO	NAPRIN	ARCRD	GEORD

COMMON: FORCE

DISPLY GPRDR

COMMON: GEOM

DRAWII	EDIT	GIPOUT	MMIOUT	MNDMOV
MNDOUT	MOVE	ROTATE	XYZMND	XYZMOV
NAAPSE	NAMODI			

COMMON: GEOSYM

GETSYM

COMMON: INTCOR

DRAWII	EDIT	GENCOR	MNDMOV	MNDOUT
XYZMND				

COMMON: KEYS

DRAWII	GENCOR	GIPOUT	INFO	MMIOUT
MNDOUT	GIPRD	GPRDR		

COMMON: KEYWRD

GETSYM

COMMON: LEGEND

DRAWII	EDIT	GIPOUT	INFO	MMIOUT
LDRAW	NAPRIN	DORTEP	PTOPEN	

COMMON: LINES

EDIT	LATOM	LBOND	LDRAW

COMMON: NAINTE

DRAWII	NAAPSE	NACIDI	NACLDI	NALIDI
NAMODI	NAPOCA			

COMMON: NAREAL

NAAPSE	NAARC	NACIDI	NACILI	NACIRC
NACSCA	NALIDI	NAMODI	NAPARM	NAPOCA
NATTHE	NAXYIN			

COMMON: OLAP

LAP500	LAP700	LAP800	LAPAB	LAPDRW

COMMON: ORBITS

DISPLY

COMMON: OUTPUT

DRAWII	DISPLY	TK4025	TERAK	TK4105
PTIGER	CONTUR			

COMMON: PLOTS

HALPLT	MINMAX	PLOT	TK4025	TERAK
TK4105	PTIGER	LDRAW	NAMODI	DRELIM
CONTUR				

COMMON: PTIGER

PTCLR	PTDOT	PTLABL	PTOUT

COMMON: STRING

BOND	F700	F900	DORTEP	DRELIM
SEARC				

COMMON: TK41XX

TK4105 TEKCRD

COMMON: TKSCRN

INFO TK4105

COMMON: VALNCE

DRAWII EDIT INFO

COMMON: VANRAD

DRAWII EDIT INFO MMIOUT LBOND
NAAPSE DORTEP DRELIM

APPENDIX C

FORTRAN FILES

The following FORTRAN-77 files constitute DRAW version 2.00.

ARCRD	ATDIST	AXIS	BANGLE	BITMAP	BPDBRD
CLEAN	CONTOUR	CORRD	DANG	DEC240	DIHED
DISPLAY	DRAW2	DTERAK	EDIT	EDITAD	EDITCH
EDITIN	ELEMNT	EPSON	GEORD	GETIC	GETSYM
GIGI	GIPOUT	GIPRD	GMETRY	GPRDR	GROUPS
GTEXT	HALPLT	HELP	HQRII	INFO	IRCRD
LA50	LARROW	LCLEAN	LINE	MATIN	MINMAX
MMIOUT	MNDMOV	MNDOUT	MOVE	MPI99	NAGOYA
NAPRIN	NUCHAR	ORTEP	OUTPLT	PICTURE	PLOT
PTIGER	QUIT	RCART	READA	READER	RETROG
REULR	ROTATE	ROTSUM	RPAIR	SETLAB	SETTRM
SETVEC	SIMBOL	TEMP	TERAK	TIGER	TK4010
TK4025	TK4105	TOTROT	UPCASE	UPROMP	VECRED
WRITE	XYZMND	XYZMOV			

APPENDIX D

STRUCTURE FILES

Your distribution tape for DRAW also includes a number of special data files. These data files contain structures of various molecules, functional groups, and prosthetic groups. These structures are designed for use by the EDIT MERGE facility. A full description of this facility is contained in the chapter on commands and in the chapter in editing.

Here is a list of the structures available at the time this manual was written. For a complete list of the structures in your distribution kit, look for all files with the extension ".DRW". You can write any additional files in your distribution at the end of the following list. For each of the files in this listing, I have included a full listing of the actual files starting on the next page of this appendix.

MERGE STRUCTURE FILES

ADENINE - DNA base unit ADENINE (without the sugar)
AIBZZ - Alpha-aminoisobutyric acid a BLOCKING GROUP
ALAZZ - Alanine, zwitter ion
ARGZZ - Arginine, zwitter ion
ASNZZ - Asparagine, zwitter ion
ASPZZ - Aspartic acid, zwitter ion
BOCAN - Tert-butyloxycarbonyl a BLOCKING GROUP
C6BOAT - Boat form of cyclohexane
C6CHAIR - Chair form of cyclohexane
GUANINE - DNA base unit GUANINE (without the sugar)
CYSZZ - Cysteine, zwitter ion
CYTOSINE - DNA base unit CYTOSINE (without the sugar)
GLNZZ - Glutenine, zwitter ion
GLUZZ - Glutamine, zwitter ion
GLYZZ - Glycine, zwitter ion
HISZZ - Histadine, zwitter ion
ILEZZ - Isoleucine, zwitter ion
LEUZZ - Leucine, zwitter ion
LYSCA - Lysine, zwitter ion (with both N's protonated)

METZZ	- Methionine, zwitter ion
PHENYL	- Phenyl group
PHEZZ	- Phenanthrine, zwitter ion
PROZZ	- Proline, zwitter ion
SERZZ	- Serine, zwitter ion
THRZZ	- Threonine, zwitter ion
THYMINE	- DNA base unit THYMINE (without the sugar)
TRPZZ	- Tryptophane, zwitter ion
TYRZZ	- Tyrosine, zwitter ion
VALZZ	- Valine, zwitter ion

```
    T30M AM1 PRECISE
    ADENINE   BASE UNIT -A-
    ADENINE.DRW
 N     0.000000    0     0.000000    0     0.000000    0  0    0    0
 C     1.352629    1     0.000000    0     0.000000    0  1    0    0
 N     1.360417    1   130.265934    1     0.000000    0  2    1    0
 C     1.375836    1   117.583602    1     0.108724    1  3    2    1
 C     1.436685    1    87.785167    1     0.060112    1  4    2    1
 C     1.459058    1    56.952858    1     0.004961    1  5    2    1
 N     1.401877    1   166.849890    1     0.070951    1  5    2    1
 C     1.342091    1    96.381567    1     0.024339    1  7    2    1
 N     1.398687    1   164.394493    1     0.073416    1  6    2    1
 N     1.368413    1   151.977586    1  -179.665060    1  4    2    1
 H     1.112076    1   114.482039    1   179.942356    1  2    3    1
 H     0.988798    1   119.018647    1  -179.696745    1 10    4    2
 H     0.988869    1   120.893361    1    -0.712767    1 10    4    2
 H     1.096405    1   168.645698    1    -0.114760    1  8    2    1
 H     0.984874    1   116.661768    1     0.042427    1  9    2    1
 0     0           0     0           0     0           0  0    0    0
```

```
  T30M  PRECISE  AM1
  ALPHA-AMINOISOBUTYRIC ACID   (AIB)  BLOCKING GROUP
PSEUDO-AMINOACID
  AIBZZ.DRW
 N     0.000000    0     0.000000    0     0.000000    0  0    0    0
 C     1.511218    1     0.000000    0     0.000000    0  1    0    0
 C     1.623990    1   107.972440    1     0.000000    0  2    1    0
 O     1.239976    1   114.976190    1   175.445248    1  3    2    1
 O     1.258785    1   114.603991    1    -4.815531    1  3    2    1
 C     1.517755    1   108.323680    1    54.954517    1  2    3    4
 H     1.047600    1   105.720052    1     8.650107    1  1    2    3
 H     1.015167    1   111.215531    1   127.975756    1  1    2    3
 H     1.016036    1   110.577059    1  -109.479948    1  1    2    3
 C     1.518609    1   107.604605    1   -64.728077    1  2    3    4
 H     1.121024    1   107.112392    1  -172.041478    1  6    2    1
 H     1.116973    1   111.582599    1   -54.426473    1  6    2    1
 H     1.116194    1   111.806247    1    68.458348    1  6    2    1
 H     1.120570    1   107.160807    1    54.316381    1 10    2    3
 H     1.116461    1   111.788711    1   173.734056    1 10    2    3
 H     1.116889    1   111.502446    1   -63.475599    1 10    2    3
 0     0           0     0           0     0           0  0    0    0
```

```
     T600M  AM1  PRECISE
      ALANINE ZWITTER ION (AMINO ACID  ALA)
     ALAZZ.DRW
N     0.000000   0    0.000000   0    0.000000   0  0  0  0
C     1.497069   1    0.000000   0    0.000000   0  1  0  0
C     1.608825   1  108.949069   1    0.000000   0  2  1  0
O     1.239914   1  114.949678   1  174.286036   1  3  2  1
O     1.260206   1  114.566738   1   -5.064077   1  3  2  1
C     1.509667   1  109.274597   1  -61.952075   1  2  3  4
H     1.051360   1  105.644784   1    6.037603   1  1  2  3
H     1.016078   1  111.342357   1  124.868558   1  1  2  3
H     1.014871   1  111.045700   1 -112.247227   1  1  2  3
H     1.124139   1  107.125947   1   57.686680   1  2  3  4
H     1.121481   1  106.957835   1  175.204743   1  6  2  1
H     1.116347   1  112.054606   1  -65.359117   1  6  2  1
H     1.117090   1  111.643911   1   57.430545   1  6  2  1
0     0          0    0          0    0          0  0  0  0
```

T30M AM1 PRECISE
ARGININE ZWITTERION (AMINOACID ARG)
ARGZZ.DRW

N	0.000000	0	0.000000	0	0.000000	0	0	0	0
C	1.495227	1	0.000000	0	0.000000	0	1	0	0
C	1.610964	1	108.834846	1	0.000000	0	2	1	0
O	1.240141	1	115.193256	1	-172.188921	1	3	2	1
O	1.259374	1	114.289945	1	8.802840	1	3	2	1
H	1.014335	1	111.732339	1	-134.346500	1	1	2	3
H	1.017810	1	110.462564	1	103.249795	1	1	2	3
H	1.124709	1	106.425863	1	72.052237	1	2	3	4
H	1.049545	1	105.690815	1	-14.394811	1	1	2	3
C	1.514800	1	109.780628	1	124.603548	1	2	3	1
C	1.512323	1	112.853249	1	-68.351127	1	10	2	1
C	1.529284	1	109.673624	1	-173.994888	1	11	10	2
N	1.452168	1	112.377225	1	179.206131	1	12	11	10
C	1.457168	1	112.786802	1	176.901059	1	13	12	11
N	1.308247	1	119.341910	1	-103.377149	1	14	13	12
N	1.421098	1	114.679089	1	81.966568	1	14	13	12
H	1.128146	1	105.712167	1	49.049051	1	10	2	3
H	1.122282	1	110.717269	1	-66.018014	1	10	2	3
H	1.122086	1	110.281950	1	65.073746	1	11	10	2
H	1.121951	1	109.928723	1	-53.253217	1	11	10	2
H	1.127398	1	108.508051	1	59.879276	1	12	11	10
H	1.129945	1	108.311972	1	-56.354506	1	12	11	10
H	1.004591	1	111.108047	1	52.161598	1	13	12	11
H	0.995973	1	116.300821	1	-174.418815	1	15	14	13
H	0.993758	1	115.133848	1	-148.825667	1	16	14	13
H	0.993867	1	116.603725	1	-10.984177	1	16	14	13
0	0	0	0	0	0	0	0	0	0

```
      T600M  AM1  PRECISE
       ASPARAGINE  ZWITTERION  (AMINOACID  ASN)
      ASNZZ.DRW
N      0.000000   0     0.000000   0     0.000000   0  0   0   0
C      1.495637   1     0.000000   0     0.000000   0  1   0   0
C      1.609177   1   108.978726   1     0.000000   0  2   1   0
O      1.243558   1   114.972434   1   176.526440   1  3   2   1
O      1.256620   1   114.890155   1    -3.210420   1  3   2   1
H      1.017602   1   111.788618   1   128.072356   1  1   2   3
H      1.048699   1   106.115244   1     8.376291   1  1   2   3
H      1.125440   1   106.787354   1  -115.741982   1  2   3   1
H      1.016599   1   110.475475   1  -109.490131   1  1   2   3
C      1.522119   1   109.539554   1   124.196731   1  2   3   1
H      1.123857   1   109.353496   1   104.619606   1 10   2   1
H      1.122771   1   113.084525   1   -15.403343   1 10   2   1
C      1.523705   1   110.295796   1  -134.887161   1 10   2   1
O      1.251304   1   119.930990   1   113.152575   1 13  10   2
N      1.361731   1   117.990943   1   -67.083154   1 13  10   2
H      0.989139   1   119.685455   1  -179.232402   1 15  13  10
H      0.997142   1   120.654465   1     3.388730   1 15  13  10
0      0          0     0          0     0          0  0   0   0
```

```
      T30M  AM1  PRECISE
       ASPARTIC ACID  ZWITTERION  (AMINOACID ASP)
      ASPZZ.DRW
N      0.000000   0     0.000000   0     0.000000   0  0   0   0
C      1.491809   1     0.000000   0     0.000000   0  1   0   0
C      1.624234   1   109.087474   1     0.000000   0  2   1   0
O      1.238543   1   114.143354   1   173.297670   1  3   2   1
O      1.255782   1   114.180886   1    -6.702461   1  3   2   1
H      1.020293   1   111.739870   1   134.410140   1  1   2   3
H      1.045935   1   106.187388   1    14.157297   1  1   2   3
H      1.123351   1   107.170807   1  -117.219187   1  2   3   1
H      1.016294   1   110.146294   1  -103.495209   1  1   2   3
C      1.513633   1   107.394972   1   124.047160   1  2   3   1
H      1.131086   1   106.368279   1   173.181690   1 10   2   1
H      1.123949   1   111.241921   1    56.437890   1 10   2   1
C      1.493392   1   114.691841   1   -66.785034   1 10   2   1
O      1.229919   1   129.555412   1  -131.100132   1 13  10   2
O      1.373142   1   114.753488   1    50.282973   1 13  10   2
H      0.971131   1   131.904750   1   165.105843   1 15  11  10
0      0          0     0          0     0          0  0   0   0
```

T30M AM1 PRECISE
TERT-BUTYLOXYCARBONYL (BOC)
BOCAN.DRW TERMINAL GROUP REF: JACS 1983 1 105-109

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	
C	1.525218	1	0.000000	0	0.000000	0	1	0	0	
C	1.518977	1	110.888284	1	0.000000	0	2	1	0	
C	1.518991	1	111.533820	1	124.110715	1	2	3	1	
O	1.456347	1	110.004167	1	-113.512174	1	2	3	1	
C	1.354192	1	119.507154	1	179.804634	1	5	2	1	
O	1.224419	1	97.249876	1	179.705170	1	6	2	1	
H	1.115341	1	108.936677	1	61.191051	1	1	2	3	
H	1.115585	1	110.256797	1	-178.833797	1	1	2	3	
H	1.115659	1	110.245566	1	-58.783963	1	1	2	3	
H	1.115653	1	109.411327	1	-60.947535	1	3	2	1	
H	1.116003	1	110.219151	1	58.901743	1	3	2	1	
H	1.117599	1	110.309174	1	179.150695	1	3	2	1	
H	1.116042	1	110.213832	1	-59.878213	1	4	2	1	
H	1.115659	1	109.399491	1	59.964235	1	4	2	1	
H	1.117589	1	110.325472	1	179.886874	1	4	2	1	
O	1.349749	1	141.190121	1	-0.325257	1	6	2	1	
H	0.972586	1	84.656906	1	-0.239236	1	17	2	1	
0	0	0	0	0	0	0	0	0	0	

T600M PRECISE
C6 BOAT CONFORMATION: AX H9, H8, H12, H14, H15; AX H18 REMOVED
C6BOAT.DRW

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	
C	1.540228	1	0.000000	0	0.000000	0	1	0	0	
C	1.539028	1	115.535220	1	0.000000	0	2	1	0	
C	1.537174	1	115.074366	1	-17.203835	1	1	2	3	
C	1.539400	1	114.835933	1	48.344786	1	4	1	2	
C	1.540201	1	115.542877	1	-29.758184	1	5	4	1	
H	1.114142	1	109.219796	1	105.250063	1	2	1	4	
H	1.114210	1	108.563956	1	-140.154274	1	2	1	4	
H	1.114483	1	109.300378	1	92.365170	1	3	2	1	
H	1.114071	1	108.905803	1	-152.787986	1	3	2	1	
H	1.113937	1	108.792012	1	170.653377	1	4	1	2	
H	1.114663	1	109.135812	1	-74.660304	1	4	1	2	
H	1.114218	1	109.117865	1	92.864809	1	5	4	1	
H	1.114081	1	108.374837	1	-152.697[illegible]	1	5	4	1	
H	1.114429	1	109.127423	1	104.7[illegible]	1	6	5	4	
H	1.113930	1	109.040354	1	-140.3[illegible]	1	6	5	4	
H	1.113825	1	109.059003	1	-139.568247	1	1	2	3	
0	0	0	0	0	0	0	0	0	0	

T600M PRECISE
C6 CHAIR CONFORMATION: AXIAL H ARE 7, 10, 16, 13, 12, 17
C6CHAIR.DRW

C	0.000000	0	0.000000	0	0.000000	0	0	0	0
C	1.538421	1	0.000000	0	0.000000	0	1	0	0
C	1.538282	1	114.052065	1	0.000000	0	2	1	0
C	1.538138	1	114.084149	1	-46.576001	1	1	2	3
C	1.538605	1	114.148803	1	46.343142	1	4	1	2
C	1.538430	1	114.178979	1	-46.019847	1	5	4	1
H	1.114269	1	109.411346	1	76.330259	1	2	1	4
H	1.113777	1	108.946919	1	-168.532342	1	2	1	4
H	1.113806	1	108.939898	1	168.437420	1	3	2	1
H	1.114220	1	109.397111	1	-76.445856	1	3	2	1
H	1.113822	1	108.941468	1	168.327486	1	4	1	2
H	1.114337	1	109.387895	1	-76.535780	1	4	1	2
H	1.114313	1	109.366536	1	76.875320	1	5	4	1
H	1.113770	1	108.925497	1	-168.022228	1	5	4	1
H	1.113849	1	108.905611	1	167.905300	1	6	5	4
H	1.114284	1	109.382896	1	-77.001389	1	6	5	4
H	1.114381	1	109.385322	1	76.320861	1	1	2	3
H	1.113767	1	108.952982	1	-168.558050	1	1	2	3
0	0	0	0	0	0	0	0	0	0

T30M PRECISE AM1
CYSTEINE ZWITTER ION (AMINOACID CYS)
CYSZZ.DRW

N	0.000000	0	0.000000	0	0.000000	0	0	0	0
C	1.491517	1	0.000000	0	0.000000	0	1	0	0
C	1.616166	1	108.232446	1	0.000000	0	2	1	0
O	1.241413	1	115.332398	1	-155.271049	1	3	2	1
O	1.255838	1	113.774859	1	24.633322	1	3	2	1
H	1.014185	1	112.100062	1	-147.091493	1	1	2	3
H	1.026300	1	108.899869	1	90.820411	1	1	2	3
H	1.125348	1	105.765579	1	89.042841	1	2	3	4
C	1.510882	1	111.327743	1	-30.288345	1	2	3	4
S	1.737608	1	111.927082	1	-71.300859	1	9	2	3
H	1.119569	1	107.802953	1	48.354797	1	9	2	3
H	1.114553	1	112.954427	1	170.639773	1	9	2	3
H	1.334260	1	98.825269	1	73.338965	1	10	9	2
H	1.042895	1	105.999538	1	-26.300632	1	1	2	3
0	0	0	0	0	0	0	0	0	0

```
     T600M  AM1  PRECISE
      BASE UNIT  CYTOSINE  -C-
     CYTOSINE.DRW
C     0.000000   0    0.000000   0    0.000000   0  0   0   0
C     1.465565   1    0.000000   0    0.000000   0  1   0   0
N     1.347637   1  122.274219   1    0.000000   0  2   1   0
C     1.400106   1  118.492644   1    0.041374   1  3   2   1
N     1.440244   1  120.155538   1   -0.046813   1  4   3   1
C     1.371611   1  117.779827   1   -0.006733   1  1   2   3
N     1.373603   1  119.517882   1 -179.780901   1  2   3   1
O     1.246975   1  123.924821   1  179.994453   1  4   3   1
H     1.094097   1  121.026849   1 -179.965815   1  1   2   3
H     0.989708   1  120.998715   1  179.341852   1  7   2   1
H     0.986566   1  119.150109   1    1.436988   1  7   2   1
H     0.993948   1  118.548000   1  179.984514   1  5   4   1
H     1.106676   1  121.514606   1  179.968496   1  6   1   2
0     0          0    0          0    0          0  0   0   0

     T600M  PRECISE  AM1
     GLUTAMINE ZWITTERION (AMINOACID GLN)
     GLNZZ.DRW
N     0.000000   0    0.000000   0    0.000000   0  0   0   0
C     1.495820   1    0.000000   0    0.000000   0  1   0   0
C     1.607391   1  109.278187   1    0.000000   0  2   1   0
O     1.241386   1  115.176443   1 -174.890536   1  3   2   1
O     1.259336   1  114.635865   1    5.417691   1  3   2   1
C     1.516969   1  113.158925   1 -123.277102   1  2   1   3
C     1.515639   1  112.524493   1   71.696089   1  6   2   1
C     1.517460   1  109.484879   1 -132.980401   1  7   6   1
O     1.251215   1  105.053271   1  -44.973087   1  8   2   1
N     1.367972   1  130.532791   1  157.977738   1  8   2   1
H     1.018848   1  110.776862   1  112.081803   1  1   2   3
H     1.048937   1  105.898582   1   -6.330302   1  1   2   3
H     1.125173   1  107.650295   1  115.336746   1  2   1   3
H     1.125694   1  105.946199   1 -169.498910   1  6   2   1
H     1.122785   1  111.329243   1  -52.383069   1  6   2   1
H     1.121681   1   87.263610   1   19.290271   1  7   2   1
H     1.123811   1   95.745490   1  126.291960   1  7   2   1
H     0.987456   1   86.944336   1  135.179799   1 10   2   1
H     0.989548   1  149.796807   1  -73.727361   1 10   2   1
H     1.014808   1  111.372288   1 -125.606011   1  1   2   3
0     0          0    0          0    0          0  0   0   0
```

T600M AM1 PRECISE CHARGE-1
GLUTAMIC ACID ZWITTERION (GLU) (ACID FUNCTION IONIZED)
GLUZZ.DRW

N	0.000000	0	0.000000	0	0.000000	0	0	0	0
C	1.457268	1	0.000000	0	0.000000	0	1	0	0
C	1.567900	1	113.468820	1	0.000000	0	2	1	0
O	1.264483	1	117.348264	1	-31.435400	1	3	2	1
C	1.533158	1	112.326965	1	-122.663056	1	2	1	3
C	1.515184	1	113.457625	1	57.920035	1	5	2	1
C	1.496281	1	116.758390	1	-34.878529	1	6	2	1
O	1.238502	1	166.513546	1	153.561115	1	7	2	1
O	1.361851	1	80.571102	1	-33.826532	1	7	2	1
O	1.258560	1	117.225551	1	148.743506	1	3	2	1
H	1.129873	1	77.654520	1	70.248743	1	6	2	1
H	1.122684	1	137.318564	1	172.094903	1	6	2	1
H	1.122792	1	106.307929	1	177.520459	1	5	2	1
H	1.121586	1	110.162011	1	-66.057412	1	5	2	1
H	1.128147	1	108.608903	1	119.256870	1	2	1	3
H	2.081333	1	101.459512	1	131.276582	1	1	2	3
H	1.008585	1	108.052447	1	32.814907	1	1	2	3
H	1.001525	1	108.899013	1	-83.344110	1	1	2	3
0	0	0	0	0	0	0	0	0	0

T30M AM1 PRECISE
GLYCINE ZWITTERION (AMINOACETIC ACID, GLY)
GLYZZ.DRW

N	0.000000	0	0.000000	0	0.000000	0	0	0	0
C	1.482685	1	0.000000	0	0.000000	0	1	0	0
C	1.594448	1	109.850795	1	0.000000	0	2	1	0
O	1.239711	1	115.121139	1	174.849954	1	3	2	1
O	1.261883	1	114.371327	1	-5.247739	1	3	2	1
H	1.055201	1	105.394715	1	7.712874	1	1	2	3
H	1.015893	1	111.227752	1	-110.048023	1	1	2	3
H	1.118438	1	108.834112	1	54.236722	1	2	3	4
H	1.119003	1	108.109877	1	-65.368813	1	2	3	4
H	1.014916	1	111.915427	1	126.834229	1	1	2	3
0	0	0	0	0	0	0	0	0	0

```
      T600M  AM1  PRECISE
       GUANINE   BASE UNIT -G-
      GUANINE.DRW
N     0.000000  0    0.000000  0    0.000000  0  0  0  0
C     1.355643  1    0.000000  0    0.000000  0  1  0  0
N     1.409279  1  124.509134  1    0.000000  0  2  1  0
C     1.422756  1  122.854375  1   -2.858962  1  3  2  1
C     1.448335  1  113.872193  1    0.049361  1  4  3  1
C     1.383157  1  114.223670  1    2.968396  1  1  2  3
N     1.395739  1  110.306355  1 -179.556103  1  5  6  1
C     1.346152  1  104.884090  1   -0.246152  1  7  5  1
N     1.394678  1  105.675588  1  179.500943  1  6  5  1
N     1.413202  1  118.245957  1 -174.160968  1  2  1  6
O     1.238830  1  117.548394  1 -179.025170  1  4  3  2
H     0.997704  1  136.696704  1  162.021793  1 10  4  3
H     0.995494  1   98.562248  1   22.291525  1 10  4  3
H     1.095331  1  125.470888  1  179.926264  1  8  7  5
H     0.985139  1  126.452426  1   -0.674925  1  9  6  1
H     0.996975  1  120.042062  1 -177.243298  1  3  2  1
0     0         0    0         0    0         0  0  0  0
```

```
      T600M  AM1  PRECISE
      HISTADINE  ZWITTERION  (AMINOACID  HIS)
      HISZZ.DRW
N     0.000000  0    0.000000  0    0.000000  0  0  0  0
C     1.493276  1    0.000000  0    0.000000  0  1  0  0
C     1.612661  1  108.919076  1    0.000000  0  2  1  0
O     1.239597  1  114.626238  1  166.252435  1  3  2  1
O     1.257410  1  114.227709  1  -14.023267  1  3  2  1
H     1.019891  1  111.583130  1  145.190256  1  1  2  3
H     1.043343  1  106.088382  1   24.305601  1  1  2  3
H     1.123083  1  108.622927  1   48.519784  1  2  3  4
H     1.017056  1  109.776253  1  -92.576481  1  1  2  3
C     1.520428  1  107.372551  1  122.858564  1  2  3  1
C     1.476317  1  112.841307  1  -50.381957  1 10  2  1
N     1.400097  1  150.687791  1   79.899898  1 11  2  1
C     1.398510  1  122.179816  1  -61.007790  1 12  2  1
N     1.351333  1   69.100292  1  -73.697495  1 13  2  1
C     1.391142  1   14.641837  1 -113.572966  1 14  2  1
H     1.128212  1  106.209955  1 -171.349438  1 10  2  1
H     1.125056  1  109.434867  1   73.642792  1 10  2  1
H     0.986026  1  110.176055  1  112.084493  1 12  2  1
H     1.095516  1  163.273157  1   81.397204  1 13  2  1
H     1.088886  1   76.418684  1  -84.161207  1 15  2  1
0     0         0    0         0    0         0  0  0  0
```

```
     T600M  AM1  PRECISE
      ISOLEUCINE  ZWITTERION  (AMINOACID  ILE)
     ILEZZ.DRW
N     0.000000    0     0.000000    0     0.000000    0  0    0    0
C     1.494906    1     0.000000    0     0.000000    0  1    0    0
C     1.607639    1   108.81[illegible]48   1     0.000000    0  2    1    0
O     1.240529    1   115.0014[illegible]   1  -168.273696    1  3    2    1
O     1.260217    1   114.608[illegible]    1    11.293121    1  3    2    1
C     1.526930    1   109.1[illegible]360   1    67.961322    1  2    3    4
C     1.513999    1   111.[illegible]       1   -55.255774    1  6    2    1
C     1.520449    1   111.392110            1    70.798382    1  6    2    1
H     1.015264    1   110.6[illegible]      1   101.886991    1  1    2    3
H     1.016922    1   111.347498            1  -135.230498    1  1    2    3
H     1.123977    1   [illegible]           1   -[illegible]    1  2    3    4
H     1.132559    1   [illegible]           1   -[illegible]    1  6    2    1
H     1.119609    1   [illegible]           1    -[illegible]   1  7    6    2
H     1.117117    1   111.63[illegible]     1    79.313845    1  7    6    2
H     1.117087    1   [illegible]           1  -161.126734    1  7    6    2
H     1.122813    1   [illegible]           1    [illegible]    1  8    6    2
H     1.122475    1   110.[illegible]       1   -74.509034    1  8    6    2
C     1.514673    1   111.[illegible]       1   164.942031    1  8    6    2
H     1.048503    1   [illegible]           1   -[illegible]    1  1    2    3
H     1.122341    1   [illegible]           1   [illegible]    1 18    8    6
H     1.122268    1   [illegible]           1   [illegible]    1 18    8    6
C     1.506931    1   [illegible]           1  -[illegible]    1 18    8    6
H     1.116823    1   [illegible]           1   -[illegible]   1 22   18    8
H     1.116932    1   [illegible]           1   [illegible]    1 22   18    8
H     1.116852    1   [illegible]           1   -[illegible]   1 22   18    8
0     0                                                       0  0    0    0
```

```
     T600M  AM1  PRECISE
      LEUCINE  ZWITTERION  (AMINOACID  LEU)
     LEUZZ.DRW
N     0.000000   0     0.000000   0     0.000000   0  0  0  0
C     1.495397   1     0.000000   0     0.000000   0  1  0  0
C     1.606450   1   108.908798   1     0.000000   0  2  1  0
O     1.240565   1   115.080008   1   168.808037   1  3  2  1
O     1.260599   1   114.629273   1   -10.610595   1  3  2  1
C     1.526866   1   113.195064   1  -121.817484   1  2  1  3
C     1.512739   1   111.468865   1   -70.681407   1  6  2  1
C     1.522558   1   111.919120   1    55.168869   1  6  2  1
H     1.017037   1   111.291161   1   131.570054   1  1  2  3
H     1.015044   1   110.877912   1  -105.565041   1  1  2  3
H     1.124213   1   108.298745   1   116.499233   1  2  1  3
H     1.132513   1   104.226706   1   171.980240   1  6  2  1
H     1.116897   1    88.842321   1  -110.811746   1  7  2  1
H     1.117198   1    95.530535   1    -2.231819   1  7  2  1
H     1.117553   1   144.038248   1   128.790791   1  7  2  1
H     1.125549   1    80.451991   1    82.992833   1  8  2  1
H     1.122607   1   102.298459   1   -23.315441   1  8  2  1
C     1.507388   1   141.737388   1  -168.285589   1  8  2  1
H     1.116740   1   105.593347   1   -94.523740   1 18  2  1
H     1.116968   1   132.117733   1    39.479833   1 18  2  1
H     1.117334   1    91.302653   1   155.921570   1 18  2  1
H     1.049276   1   105.727360   1    12.446402   1  1  2  3
0     0          0     0          0     0          0  0  0  0
```

```
     T600M  AM1  PRECISE
      METHIONINE  ZWITTERION  (AMINOACID  MET)
      METZZ.DRW
 N    0.000000   0    0.000000   0    0.000000   0  0   0   0
 C    1.495630   1    0.000000   0    0.000000   0  1   0   0
 C    1.611355   1  108.856937   1    0.000000   0  2   1   0
 O    1.240133   1  115.204735   1 -171.237284   1  3   2   1
 O    1.259217   1  114.251895   1    9.767975   1  3   2   1
 H    1.014417   1  111.685308   1 -131.869973   1  1   2   3
 H    1.018068   1  110.601647   1  105.657363   1  1   2   3
 H    1.124660   1  106.180661   1   73.100869   1  2   3   4
 H    1.050548   1  105.701455   1  -12.220620   1  1   2   3
 C    1.516236   1  110.215237   1  -46.524313   1  2   3   4
 C    1.506808   1  112.203344   1  162.572633   1 10   2   3
 S    1.737649   1  112.438290   1  169.201681   1 11  10   2
 C    1.727796   1  103.033055   1   74.334044   1 12  11  10
 H    1.129282   1  105.901043   1   41.959626   1 10   2   3
 H    1.122880   1  111.023328   1  -73.153094   1 10   2   3
 H    1.115700   1  111.996944   1   53.297725   1 11  10   2
 H    1.115730   1  111.083073   1  -69.321746   1 11  10   2
 H    1.110369   1  109.618791   1   61.902049   1 13  12  11
 H    1.111067   1  105.167724   1 -178.933137   1 13  12  11
 H    1.110796   1  109.797696   1  -59.718302   1 13  12  11
 0    0          0    0          0    0          0  0   0   0
```

```
   PRECISE  MNDO
   PHENYL.DRW
   INTENDED ATTACHMENT IS VIA CARBON C1 WHERE THE H HAS BEEN
REMOVED
 C    0.000000   0    0.000000   0    0.000000   0  0   0   0
 C    1.406653   1    0.000000   0    0.000000   0  1   0   0
 C    1.406614   1  119.963826   1    0.000000   0  2   1   0
 C    1.406519   1  120.018908   1   -0.046700   1  1   2   3
 C    1.406559   1  120.015101   1    0.055738   1  4   1   2
 C    1.406618   1  119.976432   1   -0.039290   1  5   4   1
 H    1.090299   1  120.018313   1  179.974121   1  2   3   1
 H    1.090326   1  119.989450   1 -179.988385   1  3   2   1
 H    1.090276   1  119.996048   1 -179.995512   1  6   3   1
 H    1.090354   1  119.987466   1 -179.963663   1  4   1   2
 H    1.090315   1  120.006504   1  179.973744   1  5   4   1
 0    0          0    0          0    0          0  0   0   0
```

```
     T600M  AM1  PRECISE
      PHENYLALANINE  ZWITTERION  (AMINOACID PHE)
     PHEZZ.DRW
N     0.000000   0    0.000000   0    0.000000   0  0   0   0
C     1.495356   1    0.000000   0    0.000000   0  1   0   0
C     1.606543   1  109.272036   1    0.000000   0  2   1   0
O     1.240432   1  114.847019   1  172.025477   1  3   2   1
O     1.259288   1  114.551399   1   -7.639737   1  3   2   1
H     1.015350   1  110.627726   1 -105.920823   1  1   2   3
H     1.019332   1  111.114270   1  131.735446   1  1   2   3
H     1.123624   1  108.142717   1  117.332395   1  2   1   3
H     1.047473   1  105.919034   1   12.056493   1  1   2   3
C     1.521390   1  112.573237   1 -120.676856   1  2   1   3
H     1.126864   1  106.007199   1 -178.360340   1 10   2   1
H     1.123123   1  109.998845   1   66.512214   1 10   2   1
C     1.487817   1  112.414766   1  -57.135428   1 10   2   1
C     1.400169   1  121.681325   1   30.428390   1 13   2   1
C     1.394227   1  143.744648   1  -79.259414   1 14   2   1
C     1.394521   1   99.612974   1 -117.828280   1 15   2   1
C     1.395435   1   57.708612   1 -138.859914   1 16   2   1
C     1.400544   1  108.236464   1 -113.582884   1 13   2   1
H     1.100766   1   89.670994   1   66.930791   1 14   2   1
H     1.100257   1  137.252761   1   40.727633   1 15   2   1
H     1.100028   1  164.291909   1  -52.221027   1 16   2   1
H     1.100422   1  129.815066   1 -118.820677   1 17   2   1
H     1.101177   1   79.309281   1 -141.949149   1 18   2   1
0     0          0    0          0    0          0  0   0   0
```

```
     T600M  AM1  PRECISE
      PROLINE  ZWITTER ION (AMINOACID  PRO)
     PROZZ.DRW
N     0.000000   0     0.000000   0     0.000000   0  0  0  0
C     1.506542   1     0.000000   0     0.000000   0  1  0  0
C     1.599785   1   109.548209   1     0.000000   0  2  1  0
O     1.241449   1   115.211391   1  -176.399145   1  3  2  1
O     1.260426   1   114.768241   1     3.999035   1  3  2  1
H     1.014909   1   110.983096   1  -115.726198   1  1  2  3
H     1.121207   1   108.772619   1   117.147111   1  2  1  3
C     1.526378   1   108.077641   1  -121.523983   1  2  1  3
C     1.523028   1   107.469454   1     2.862652   1  8  2  1
C     1.491277   1   108.672175   1   121.582552   1  1  2  3
H     1.121710   1   109.240927   1   124.062292   1  8  2  1
H     1.118549   1   110.211686   1  -118.065559   1  8  2  1
H     1.118944   1   121.389872   1   100.340303   1  9  2  1
H     1.117918   1   127.427607   1  -102.918167   1  9  2  1
H     1.124197   1   124.638100   1    73.248255   1 10  2  1
H     1.123441   1   121.607739   1   -78.602843   1 10  2  1
H     1.048492   1   105.554689   1     2.176868   1  1  2  3
0     0          0     0          0     0          0  0  0  0
```

```
     T600M  AM1  PRECISE
      SERINE ZWITTER ION (AMINOACID  SER)
     SERZZ.DRW
N     0.000000   0     0.000000   0     0.000000   0  0  0  0
C     1.488436   1     0.000000   0     0.000000   0  1  0  0
C     1.603899   1   109.130875   1     0.000000   0  2  1  0
O     1.243705   1   114.771387   1  -168.043316   1  3  2  1
O     1.257416   1   114.725519   1    12.143823   1  3  2  1
H     1.015135   1   111.654323   1  -135.975078   1  1  2  3
H     1.017823   1   110.564078   1   101.534769   1  1  2  3
H     1.124948   1   108.575277   1   115.811092   1  2  1  3
C     1.533490   1   113.499771   1  -122.026480   1  2  1  3
O     1.404634   1   109.418071   1  -160.864844   1  9  2  1
H     1.122944   1   109.702568   1    77.353225   1  9  2  1
H     1.124212   1   111.951052   1   -44.934796   1  9  2  1
H     0.974707   1    88.568444   1   153.096555   1 10  2  1
H     1.049254   1   105.720032   1   -16.100474   1  1  2  3
0     0          0     0          0     0          0  0  0  0
```

```
      T600M  AM1  PRECISE
       THREONINE  ZWITTER ION  (AMINOACID  THR)
      THRZZ.DRW
N     0.000000   0    0.000000   0    0.000000   0  0  0  0
C     1.492447   1    0.000000   0    0.000000   0  1  0  0
C     1.605543   1  109.819213   1    0.000000   0  2  1  0
O     1.241043   1  115.074585   1  177.938396   1  3  2  1
O     1.258995   1  114.474575   1   -2.617072   1  3  2  1
C     1.531160   1  112.896848   1  122.672159   1  2  1  3
C     1.515897   1  113.327126   1  -66.733639   1  6  2  1
O     1.428367   1  106.398913   1   55.074959   1  6  2  1
H     1.046457   1  106.254286   1    4.011852   1  1  2  3
H     1.015114   1  110.926628   1  123.785057   1  1  2  3
H     1.124555   1  107.925107   1 -116.696424   1  2  1  3
H     1.128654   1  106.180855   1  172.773104   1  6  2  1
H     1.119092   1   87.443988   1 -106.728913   1  7  2  1
H     1.115920   1   96.846258   1    2.390938   1  7  2  1
H     1.116492   1  142.876686   1  134.923586   1  7  2  1
H     0.963562   1  144.764141   1 -143.890277   1  8  2  1
H     1.019173   1  110.194198   1 -114.922938   1  1  2  3
0     0          0    0          0    0          0  0  0  0
```

```
      T600M AM1 PRECISE
      BASE UNIT  THYMINE  -T-
      THYMINE.DRW
C     0.000000   0    0.000000   0    0.000000   0  0  0  0
C     1.476817   1    0.000000   0    0.000000   0  1  0  0
N     1.407192   1  116.408969   1    0.000000   0  2  1  0
C     1.401630   1  122.896724   1    0.518966   1  3  2  1
N     1.412571   1  118.044512   1    0.271554   1  4  3  1
C     1.363328   1  119.701051   1   -0.685840   1  1  2  3
C     1.475249   1  117.421768   1  179.135167   1  1  2  3
O     1.249199   1  121.851560   1 -179.742808   1  4  3  1
O     1.241785   1  118.518831   1 -179.830243   1  2  3  1
H     1.117359   1  111.169359   1  157.112439   1  7  1  2
H     1.119653   1  110.083605   1  -82.465244   1  7  1  2
H     0.993868   1  117.526950   1 -179.910062   1  5  4  1
H     1.106308   1  122.234882   1 -179.607232   1  6  1  2
H     1.119603   1  110.094199   1   36.330783   1  7  1  2
H     0.997387   1  119.819262   1 -179.866737   1  3  2  1
0     0          0    0          0    0          0  0  0  0
```

```
      T600M  AM1  PRECISE
      TRYPTOPHANE  ZWITTERION (AMINO ACID TRP)
      TRPZZ.DRW
N     0.000000  0    0.000000  0    0.000000  0  0  0  0
C     1.498801  1    0.000000  0    0.000000  0  1  0  0
C     1.613892  1  106.495874  1    0.000000  0  2  1  0
O     1.238204  1  115.623447  1  144.545945  1  3  2  1
O     1.259592  1  113.385568  1  -32.883081  1  3  2  1
H     1.016056  1  112.368212  1  152.284442  1  1  2  3
H     1.044974  1  105.449287  1   32.112516  1  1  2  3
H     1.122161  1  108.262598  1  116.956129  1  2  1  3
C     1.525301  1  111.694359  1 -120.242963  1  2  1  3
C     1.467944  1  106.831756  1 -140.820730  1  9  3  1
C     1.394022  1  101.132195  1 -108.660639  1 10  2  1
N     1.398983  1  156.093776  1  153.962701  1 11  2  1
C     1.451765  1  144.827273  1  108.833793  1 10  2  1
C     1.444888  1  123.218726  1 -132.238849  1 13  2  1
C     1.394978  1  115.322183  1   63.850801  1 13  2  1
C     1.387555  1  162.191416  1  178.623138  1 15  2  1
C     1.402989  1  158.700995  1  109.671558  1 14  2  1
C     1.386896  1  103.464971  1   72.327154  1 17  2  1
H     1.128847  1  110.833101  1  -33.042684  1  9  2  1
H     1.126439  1  108.461833  1   84.366498  1  9  2  1
H     1.091350  1   79.251765  1  -60.280869  1 11  2  1
H     0.985910  1  132.004727  1  -99.716201  1 12  2  1
H     1.099459  1   72.923501  1   35.552317  1 15  2  1
H     1.099844  1  129.424156  1   46.929846  1 16  2  1
H     2.151847  1  129.516508  1   77.657405  1 17  2  1
H     2.169279  1   89.947838  1 -129.620205  1 18  2  1
H     1.016623  1  109.706549  1  -84.680967  1  1  2  3
0     0         0    0         0    0         0  0  0  0
```

```
      T600M  AM1  PRECISE
       TYROSINE   ZWITTERION  (AMINOACID  TYR)
       TYRZZ.DRW
 N     0.000000   0    0.000000   0    0.000000   0  0   0   0
 C     1.495297   1    0.000000   0    0.000000   0  1   0   0
 C     1.606330   1  109.261595   1    0.000000   0  2   1   0
 O     1.240510   1  114.825528   1  170.887766   1  3   2   1
 O     1.259212   1  114.560668   1   -8.728330   1  3   2   1
 H     1.015462   1  110.580603   1 -104.377958   1  1   2   3
 H     1.019035   1  111.162280   1  133.255171   1  1   2   3
 H     1.123590   1  108.132369   1  117.348963   1  2   1   3
 H     1.047401   1  105.920893   1   13.458880   1  1   2   3
 C     1.521552   1  112.573145   1 -120.666789   1  2   1   3
 H     1.126792   1  105.921842   1 -178.703548   1 10   2   1
 H     1.123089   1  109.991476   1   66.201485   1 10   2   1
 C     1.487249   1  112.408738   1  -57.470844   1 10   2   1
 C     1.401472   1  121.861442   1   30.303192   1 13   2   1
 C     1.390100   1  143.925983   1  -78.515842   1 14   2   1
 C     1.405483   1   98.841269   1 -117.976994   1 15   2   1
 C     1.402458   1   58.086814   1 -139.013972   1 16   2   1
 C     1.399914   1  108.180592   1 -113.964280   1 13   2   1
 H     1.101464   1   89.663207   1   66.782381   1 14   2   1
 H     1.099240   1  138.358672   1   39.913058   1 15   2   1
 O     1.374351   1  163.736301   1  -40.615845   1 16   2   1
 H     1.099367   1  130.010039   1 -118.854377   1 17   2   1
 H     1.101743   1   79.344844   1 -142.308499   1 18   2   1
 H     0.968719   1  107.975931   1 -128.435494   1 21   2   1
 0     0          0    0          0    0          0  0   0   0
```

```
T600M  AM1  PRECISE
 VALINE  ZWITTER ION (AMINOACID  VAL)
VALZZ.DRW
N    0.000000  0    0.000000  0    0.000000  0  0  0  0
C    1.494158  1    0.000000  0    0.000000  0  1  0  0
C    1.607472  1  108.976247  1    0.000000  0  2  1  0
O    1.240682  1  115.316888  1 -176.603593  1  3  2  1
O    1.260541  1  114.517042  1    4.662462  1  3  2  1
C    1.524353  1  113.616526  1 -123.483775  1  2  1  3
C    1.512159  1  111.834579  1  -68.286852  1  6  2  1
C    1.513486  1  112.647428  1   57.688365  1  6  2  1
H    1.018458  1  110.371694  1  105.954857  1  1  2  3
H    1.013980  1  111.669739  1 -131.687880  1  1  2  3
H    1.125274  1  107.606855  1  114.959155  1  2  1  3
H    1.133800  1  103.953624  1  174.148383  1  6  2  1
H    1.116767  1   89.503280  1 -109.495248  1  7  2  1
H    1.117186  1   94.909914  1   -0.889684  1  7  2  1
H    1.117300  1  143.896088  1  129.065923  1  7  2  1
H    1.118594  1   84.811575  1   92.093549  1  8  2  1
H    1.117203  1  141.415654  1 -154.602603  1  8  2  1
H    1.117260  1  101.316782  1  -16.505703  1  8  2  1
H    1.049205  1  105.784665  1  -11.620516  1  1  2  3
0    0         0    0         0    0         0  0  0  0
```