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A USER'S GUIDE TO THE MOLECULAR MODELING, ANALYSIS, AND DISPLAY SYSTEM (MMADS)

SECOND EDITION

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The Molecular Modeling, Analysis, and Display System (MMADS) provides a "chemist's workbench" - a user-friendly, integrated suite of programs organized around a common data structure. The guiding principle throughout the development of MMADS has been to provide the user with the largest practical number of programs in an environment conducive to their use. With MMADS, a tool has been constructed that incorporates application programs for quantum, physical, and physical organic chemistry, as well as state-of-the-art molecular graphics routines, in a coherent whole.

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PREFACE

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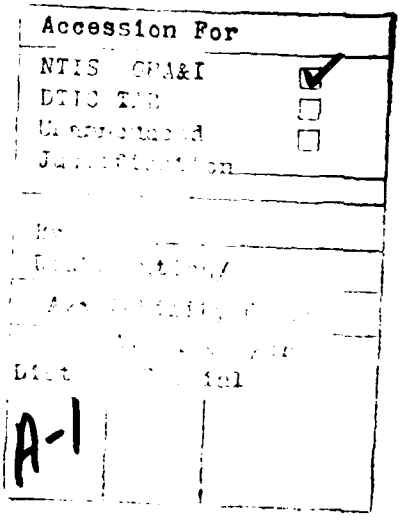

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A USER'S GUIDE TO THE MOLECULAR MODELING, ANALYSIS, AND DISPLAY SYSTEM (MMADS)

1. INTRODUCTION

The Molecular Modeling, Analysis and Display System (MMADS) provides a "chemist's workbench" - a user-friendly, integrated suite of programs organized around a common data structure. Every molecule entered into MMADS is described via a structure file. These files specify the type, location and bonding environment for each atom, along with the number of atoms in the molecule and a descriptor line for the file.

MMADS is a direct descendant of the TRIBBLE system developed by Dave Pensak at DuPont. Additional routines have been adapted from the CHEMLAB system developed by Tony Hopfinger et al at Case-Western Reserve University, the QUIPU system developed by George Purvis et al of the Quantum Theory Project at the University of Florida and the Quantum Chemistry Program Exchange (QCPE). Integration of the individual programs, and development of programs unavailable from other sources have been performed at the Chemometric/Biometric Modeling (CBM) Branch at the Chemical Research, Development and Engineering Center (CRDEC).

The guiding principle throughout the development of MMADS has been to provide the user with the largest practical number of programs in an environment conducive to their use. To this end, all non-commercial programs are candidates for inclusion. Several problems present themselves: first, when the code was developed, the initial authors had in mind a specific audience and environment which was usually rather different from that supported at CBM Branch. Second, few researchers have had the interest or resources needed to integrate software obtained from different sources, relying on familiarity with the individual routines for ease of use. Finally, many of the existing programs have fifteen year revision histories, and do not reflect the advances in programming methodology that have occurred in that time.

In some cases, vendor-supplied software is available that provides a desired capability. While the size of the equipment budget has been a limitation, purchase of general-purpose software has been unavoidable. For the remainder of cases, the developers have been able to modify or develop code that has been required to support mission-related investigations.

There is another reason for developing MMADS: software systems such as [illegible] provide a method of integrating the methodology of theoretical chemistry into the day-to-day operations of laboratory chemists. With MMADS, a tool has been constructed that incorporates quantum, physical and physical organic chemistry application programs as a coherent whole.

document supersedes CRDEC-TR-86039, "A User's Guide to the Molecular ... Analysis and Display System", May 1986, UNCLASSIFIED Report.

THE VAX/VMS ENVIRONMENT

... Branch maintains a pair of clustered Digital Equipment Corporation (DEC) VAX computers as the dedicated host for MMADS. High-resolution graphics ... are provided by an Adage 3000 raster display system (hosted by a DEC VAX-... connected to the VAX via a high-speed interface, along with a GPX graphics ... contained in one of the uVAX-II's. VT-100 compatible, Tektronix 4010 compatible ... Tektronix 4105 color terminals are directly connected to the VAX, with a modem and ... ted-pair network connection supporting remote use.

... VAX/VMS operating system provides an excellent framework for integrated ... such as MMADS. Using the DCL command language, the actual details of ... execution and data manipulation are hidden from the user. This document, ... with an on-line help facility, is all that is required to operate MMADS. The user ... however, to have an understanding of or appreciation for the capabilities and ... of the tool.

... access MMADS, the user must have a valid account on the VAX. To obtain an ..., contact the VAX System Manager. The user is reminded that DEC supplies a ... of manuals and user's guides, along with an extensive on-line help library. These ... provide all of the information needed for the general user, and should be consulted ... questions arise. Questions specific to MMADS should be referred to the developers, ... with any complaints or suggestions that come to mind.

MMADS can be viewed as a single (rather elaborate) program, functionally similar to ... VAX/VMS editor. To start a session, type "MMADS" to the DCL prompt ($). As ... VAX/VMS commands, this and all other MMADS commands can be abbreviated ... or lower case can be used. On entry, MMADS displays the current version ... and date, along with brief system notes. These should be checked periodically for ... of major revisions or additions that have occurred.

Several special characters are provided by the VAX/VMS operating system, entered by typing an individual letter with the <CTRL> key depressed:

<CTRL>S	Stop output on the user's terminal (pause).
<CTRL>Q	Start output on the user's terminal.

These are commonly used when reviewing a large body of text, to prevent the loss of text as it scrolls off the screen.

<CTRL>Z	Send an end-of-file indication to the VAX.
<CTRL>C	Cancel the current operation.
<CTRL>Y	Terminate execution of the current program.

Use of <CTRL>C or <CTRL>Y abnormally terminates the current MMADS command. The user is cautioned to check the status of all files, to prevent loss of data caused by such termination.

<CTRL>T	Provide a one-line status of the current task.

The response to this command indicates the current system (mmads), the user's terminal and current MMADS command (tt command), information on the amount of CPU time used and the number of I/O and paging operations that have occurred.

MMADS attempts to provide a reasonable default when prompting the user for information. These defaults are given in brackets, indicating the answer that will be used if a blank line is entered. Options that can be selected by the user are indicated in parentheses.

3. MMADS COMMANDS

All actions performed by MMADS are initiated by commands entered by the user. These include commands for structure entry, structure modification, structure maintenance, structure optimization, property determination, graphical display and theoretical calculations. In addition, MMADS supports a subset of the VAX/VMS

command language.

3.1 Structure Entry

These commands allow the user to enter a structure into MMADS, whether from a traditional chemical structure, fragments taken from structures already determined or data obtained from X-ray crystallography. Use of these commands ensures that the structure conforms to the internal data format used throughout MMADS. The user should check the current structure name before any of these commands are used, as the generated structure is saved in a structure file under that name.

3.1.1 KWIKDRAW

KWIKDRAW allows the user to create a structure file using a "dumb" terminal - it requires no graphical or screen-addressable capabilities in its operation. Each atom in the structure being constructed is assumed to be a carbon atom, unless explicitly changed by the user. Hydrogen atoms need not be specified, as KWIKDRAW can include them (where appropriate) when the structure file is saved on program exit. The maximum number of atoms (excluding generated hydrogens) that can be dealt with using KWIKDRAW is 300.

KWIKDRAW accepts the following commands:

Atom Generation	
CHAIN x	Create a chain of carbon atoms x atoms in length.
RING x	Create a ring containing x carbon atoms.
BRANCH x,n	Create a chain of carbon atoms x atoms in length, connected to atom n.
LINK x,n,m	Create a chain of carbon atoms x atoms in length, connected to atoms n and m.

If the parameters (x,n,m) are omitted, the user will be prompted for their values. Incorrect values, or references to missing atoms will be reported.

Structure Display	
ADRAW	Display the structure on the terminal, using the atomic symbols.
NDRAW	Display the structure on the terminal, using the atom numbers.

Use of these commands is limited to structures containing one hundred or fewer atoms.

Atom Connection	
JOIN n,m	Create a bond between atom n and m.
BREAK n,m	Remove a bond between atom n and m.

If the parameters (n,m) are omitted, the user will be prompted for their values. Incorrect values, or references to missing atoms will be reported.

Structure Modification	
CHANGE <atoms>	Change the atom symbol for the specified atom(s).
DELETE <atoms>	Delete the specified atom(s). Deleted atom numbers are NOT reused during the current KWIKDRAW session.

These commands use free-format input (with commas or dashes separating individual numbers). If the parameter <atoms> is omitted, the user will be prompted for the atoms to be changed/deleted. When executing the commands in this manner, only one atom can be dealt with at a time. Incorrect values, or references to missing atoms will be reported.

Other Commands	
LOAD file	*Load the specified structure file.* Any multiple bonding in the input file is ignored, so care must be taken to restore such bonds (via JOIN) where appropriate. The numbering scheme in the file being

	loaded is altered to conform to that currently in use.
RESET	Reinitializes KWIKDRAW, allowing the user to start over from scratch.
QUIT	Exit KWIKDRAW without creating a structure file.
HELP	Obtain help on the operation of KWIKDRAW.
EXIT	Exit KWIKDRAW normally.

Exiting **KWIKDRAW** Upon exiting KWIKDRAW normally, the user is prompted:

Add hydrogens (Y/N) [Y]:

allowing the user to specify whether hydrogen atoms will be added to complete the valence shell of each atom in the structure. KWIKDRAW indicates the number of hydrogens (zero is a reasonable number) added to the structure. If hydrogen generation is suppressed, KWIKDRAW is unable to determine the MM2 atom types, and the user is so informed. Next, KWIKDRAW prompts:

Generate coordinates (Y/N) [Y]:

allowing the user to specify whether an initial estimate of the molecular geometry should be made, and

Planar Projection (Y/N) [N]:

allowing the user to specify whether a 2-D (x,y plane; CPK coordinates) or 3-D (standard internal coordinates) molecular geometry should be generated. The user is informed that the molecular coordinates were generated. If a 2-D geometry is specified, the user is prompted:

Enter atom number:

which expects the number of the atom that is to be made non-planar, and

Enter Z-coordinate:

which expects the z-coordinate of the specified atom. Entering a blank line at the prompt for atom number terminates input. Finally, KWIKDRAW prompts:

Enter the title:

allowing the user to specify the title for the structure file being created. The user is informed that the structure file has been saved on disk.

3.1.2 SKETCH

SKETCH is a full-screen editor designed for VT-100 compatible terminals, allowing the user to sketch a molecular structure on a 80 column by 24 line terminal screen. The arrow keys are used to position the cursor at any point on the screen. Unlike the VAX/VMS editor, successive characters replace each other (i.e. the terminal is in overstrike rather than insert mode), requiring the user to exercise care to move the cursor after each character is hit.

With SKETCH, the user can also cut and paste segments of molecules together. These can be obtained from the current display, or from files containing suitable substructures. This allows the user to create libraries of molecular fragments, using these to speed up the creation process. To ensure correct operation, keep the CAPS LOCK key set on the terminal while using SKETCH.

SKETCH has two modes of operation: full-screen and command mode. In full-screen mode, the following keys are read as commands:

PF1	Enter/exit cut mode.
PF2	Paste the contents of the cut buffer at the current cursor position.
PF3	Undo the effect of the last paste operation.
<CTRL>X	Clear the screen.
<CTRL>R	Redisplay the entire screen.
<ret>	Exit to command mode.
<del>	Delete the character preceding the the current cursor position.

In command mode, the following commands are accepted:

INCLUDE	Include a fragment from a file.
HELP	Obtain help on the operation of SKETCH.
EXIT	Exit SKETCH and generate a structure file.
<ret>	Enter full-screen mode.

Cutting and Pasting

To perform a cut operation, position the cursor at the first location to be removed. Press the PF1 key to initiate the cut operation - SKETCH remains in cut mode until PF1 is struck again, at which point the highlighted fragment is placed in the cut buffer. Individual characters are marked for cutting by positioning the cursor and striking the SPACE BAR. The cut operation is cancelled by striking the <CTRL>X key, which discards the contents of the cut buffer.

To paste the contents of the cut buffer on the screen, position the cursor at the appropriate location and strike the PF2 key. The cursor position at which the cut operation was initiated will be translated to the current position. If this operation is incorrect, it can be undone by striking the PF3 key.

Including a file

Once the INCLUDE command has been issued, the user is prompted for the name of the file to be included. If the file is present, it will be overlaid on the display at the current cursor position. Care must be taken when preparing fragments to avoid mistakes due to atom overlap.

Normally, SKETCH generates molecular coordinates in the plane of the display (the x-y plane) upon exit. Rough z-coordinates can be specified using the following convention: if an atom lies below the plane of the display, place an apostrophe to the right of the atom symbol. If an atom lies above the plane, place a double quote to the right of the atom symbol. Two conditions must be observed: each atom must be surrounded by spaces, bonds (-, =, #, /, |) or above/below plane indicators and all bonds connecting atoms must be represented as straight lines.

3.1.3 CRYSTAL

CRYSTAL allows the user to create a structure file based on X-ray crystallographic data. Using the unit cell lengths and angles, the fractional coordinates provided by the X-ray analysis are converted into three dimensional cartesian coordinates, suitable for use in MMADS. The atom type (see Appendix A) and connectivity are omitted, as the X-ray

data specifies only the atom symbol and position.

X-ray data can be entered in one of two methods: from a file created with the VAX/VMS editor or directly from the user's terminal. Use of an input file is highly recommended, as it provides a means for error correction without involving a great deal of retyping. Such a file must have the filename suffix _.CRY. Assuming a data file has been created, the following procedure is followed:

Data file format

Record #1	Cols. 1-3, the number of atoms in the structure. Cols. 4-on, the title for the structure file.
All successive records use the following (free-format) input	<atom symbol> <x>,<y>,<z>

<x>, <y> and <z> are the fractional coordinates. The symbol must start in the first column, and at least one space must separate the coordinates from the symbol. Commas must be used to separate the fractional coordinates.

Program Execution

Upon entering CRYSTAL, the user is prompted:

Enter input filename [terminal]:

which expects the name of the data file prepared previously. Entering a blank line indicates the user will enter all fractional coordinates at the terminal. Next, the user is prompted:

Enter cell dimensions <a,b,c>:

which expects the three unit cell lengths (with decimal points) separated by commas, and

Enter cell angles <alpha,beta,gamma>:

which expects the three unit cell angles (in degrees, with decimal points) separated by commas. In cases where required values are omitted in the literature, the user is referred to texts defining the various types of unit cells to obtain the missing values.

If the user does not use a data file, two changes are made in this procedure:

After the unit cell values are entered, the user is prompted for the title of the structure file. The fractional coordinates are entered (using the aforementioned format) on successive lines. The user terminates input by typing <CTRL>Z.

3.1.4 GPXSKETCH

GPXSKETCH allows the user to create a structure file using the two-dimensional graphics capabilities of the DEC uVAX-II/GPX. With the mouse as a pointing device, the user enters the structure as a freehand sketch on the GPX Sketchpad (as it would be written on paper). Future versions of GPXSKETCH will include recognition and transformations involving molecular fragments, permit the use of fragment libraries and use the Distance Geometry algorithm to generate initial guess molecular coordinates.

Using GPXSKETCH, the user can rapidly create a stick representation of a particular structure. Multiple bonds are easily included, and are presented in a format that is natural to the researcher. Atoms and bonds can be moved and/or deleted, using the "point-and-click" paradigm popularized by the Apple Macintosh. Like KWIKDRAW, GPXSKETCH is capable of adding hydrogens to fill atomic valences.

Upon entering GPXSKETCH, the user is presented with three windows: the GPX Sketchpad, the Atom Type selection and the Commands selection display. The current selection in the Atom Type and Commands window is indicated by the highlighted entry. The default atom type is Carbon, and the default command is Add Atom. Each of the displays will be described below.

GPX Sketchpad

When the cursor is moved into the Sketchpad window, it changes from a pointer to a cross to provide a visual cue for the user. Depending on the current command, clicking the select button on the mouse triggers various actions:

Add Atom: Position an atom of the current atom type at the position specified by the cursor. This atom is connected by a single bond to the preceeding atom, unless the Break Atoms command was given. Multiple bonding is

indicated by double or triple clicking the mouse.

Move Atom: Move the atom at the position specified by the cursor. All bonds connected to the selected atom are then erased, and the atom will track the cursor as long as the select button is depressed. Once the user releases the select button, all bonds involving the selected atom are redrawn.

Erase: Delete the atom or bond at the position specified by the cursor. To delete a bond, click the select button near the midpoint of the bond. To delete an atom, click on the atom symbol - this will delete the atom, along with any bonds connected to the selected atom.

Atom Type

When the cursor is moved into the Atom Type window, GPXSKETCH assumes that the user intends to specify the current atom type. To make the selection, position the cursor on the appropriate atom type and click the select button. This selection will remain in effect until the cursor reenters the Atom Type window. The user can indicate a break in the molecular connectivity by clicking on Break Atoms (which resets the current atom type to Carbon).

Commands

When the cursor is moved into the Commands window, GPXSKETCH assumes that the user intends to specify the current command. To make a selection, position the cursor on the appropriate command and click the select button. This selection will remain in effect until the cursor reenters the Commands window (or until the user exits GPXSKETCH). The GPXSKETCH commands are:

Add Atom: Indicate that atoms are to be added to the structure being drawn on the Sketchpad.

Move Atom: Indicate that individual atoms are to be moved on the Sketchpad.

Erase: Indicate that atoms and/or bonds are to be removed from the Sketchpad.

Reset: Erases the Sketchpad, allowing the user to start again. Exits GPXSKETCH without creating a structure file.

Exit: Exits GPXSKETCH normally.

Upon exit, GPXSKETCH prompts the user:

Enter the title:

allowing the user to specify the title for the structure file being created, and

Add hydrogens (Y/N) [Y]:

allowing the user to specify whether hydrogen atoms will be added to complete the valence shell of each atom in the structure. Unlike KWIKDRAW, GPXSKETCH is able to determine the MM2 atom types for structures in which hydrogens are omitted.

3.1.5 SMILES

SMILES allows the user to create a structure file using the SMILES notation, as used in the Pomona College C LOG P package. Using this notation, molecules can be described in a straightforward and concise manner, typically requiring 10-40 characters to fully characterize the molecular framework. SMILES prompts the user:

INPUT:

which expects a one-line description of the molecular structure. The user is referred to the C LOG P documentation for a description of the SMILES notation. At this point, the user is prompted:

Add hydrogens (Y/N) [Y]:

allowing the user to specify whether hydrogen atoms will be added to complete the valence shell of each atom in the structure. SMILES indicates the number of hydrogens (zero is a reasonable number) added to the structure. If hydrogen generation is suppressed, SMILES is unable to determine the MM2 atom types, and the user is so informed. Next, SMILES prompts:

Generate coordinates (Y/N) [Y]:

allowing the user to specify whether an initial guess for the molecular geometry should be made, and

Planar Projection (Y/N) [N]:

allowing the user to specify whether a 2-D (x,y plane; CPK coordinates) or 3-D (standard internal coordinates) molecular geometry should be generated. The user is informed that the molecular coordinates were generated. If a 2-D geometry is specified, the user is prompted:

Enter atom number:

which expects the number of the atom that is to be made non-planar, and

Enter Z-coordinate:

which expects the z-coordinate of the specified atom. Entering a blank line at the prompt for atom number terminates input. Finally, SMILES prompts:

Enter the title:

allowing the user to specify the title for the structure file being created. The user is informed that the structure file has been saved on disk.

3.2 Structure Modification

These commands allow the user to make changes to a structure already entered into MMADS, while preserving the information necessary for compatibility with the other parts of the system. Using these commands, the user can alter the scaling of the individual coordinate axes (whether alone or in concert), center the structure at its center of mass, orient the structure along its principle axes, add hydrogens to complete the valence shell of each atom or remove all hydrogens from the structure file. In addition, the MMADS structure editor can be used to perform a number of operations on structure files.

3.2.1 EDIT

The MMADS structure editor is the general-purpose structure file manipulator. Using EDIT, the user can view the molecular environment of individual atoms, add atoms to or delete atoms from the structure, alter the bonding environment of individual atoms, alter the molecular geometry, change the title of the structure file, change the symbol and type of individual atoms and merge the contents of additional files with the current structure.

EDIT accepts the following commands:

Viewing atoms

VIEW <atoms>	Display the atom symbol, index, coordinates, type and connectivity of the specified atoms.
LIST	Display the above information for the entire molecule. The display pauses every 20 atoms, prompting the user to continue.

Adding or Deleting atoms

ADD	Add an atom to the structure. EDIT assigns the atom index, prompting the user for the atom symbol, coordinates, type and the atom to connect to. If the coordinates are unknown, entering a blank line will cause EDIT to generate standard coordinates.
DELETE <atoms>	Remove atoms from the structure. Deletion of an atom removes all bonds to that atom as well.

Atom Connection

JOIN n,m	Make a bond between atoms n and m.
BREAK n,m	Remove a bond between atoms n and m. If the parameters (n,m) are omitted, the user will be prompted for their values.

Geometry Alteration

BOND	Indicate the distance between the specified atoms. If the atoms are connected, the user is prompted for the new value.
ANGLE	Indicate the angle between the specified atoms. If the atoms are connected in the proper order, the user is prompted for the new value.
DIHEDRAL	Indicate the dihedral angle between the specified atoms. If the atoms are connected in the proper order, the user is prompted for the new value.

The order in which atoms are specified for these commands IS important. The segment of the molecule extending from the last atom entered will be moved. If ring structures are encountered, the user will be prompted for an atom to "freeze" in position (thus breaking the ring). All new values for geometric parameters must be entered with decimal points. The user should consider the nature of the trigonometric identities when puzzled by the signs of bond angles and dihedrals.

STANDARD — Alter the geometry to conform to standard bond lengths, angles and dihedrals. Ring structures can not be dealt with successfully at this time. Successive execution of this command might serve to improve the structure.

Changing atom characteristics

CHANGE <atoms> — Allow the user to alter the atom symbol, coordinates, type and connectivity of individual atoms. Entering a blank line preserves the existing value unchanged. Care must be taken when changing the connectivity to preserve the symmetry of the bonding information.

Other commands

TITLE — Indicate the current title, and prompt the user to specify a new title. A blank line preserves the current title.

MERGE — Merges the specified structure file. The user is prompted for the atom to be removed from the existing structure and from the structure being merged. These atoms must be terminal atoms, so care must be taken in their selection. EDIT then prints the new atom number for the first atom from the structure being merged. MERGE then executes the BOND, ANGLE and DIHEDRAL commands, to allow for proper orientation of the fragment being added.

QUIT — Exit EDIT without saving the current structure. This allows the user to perform editor operations without endangering existing files.

EXIT — Exit EDIT normally. The user is prompted whether the structure file name is to be changed.

HELP Obtain help on the operation of EDIT.

The VIEW, DELETE and CHANGE commands use the free-format input described previously. If the parameter <atoms> is omitted, the user will be prompted for the atoms to be viewed/changed/deleted. When executing commands in this manner, only one atom can be dealt with at a time. For all commands, incorrect values, or references to missing atoms will be reported.

3.2.2 GENHYDROGENS

GENHYDROGENS allows the user to add hydrogens to atoms having unfilled valence. This command performs the same function as the hydrogen addition routine in KWIKDRAW, and is useful in adding hydrogens to structure files generated using CRYSTAL (and lacking in non-essential hydrogens).

3.2.3 DELHYDROGENS

DELHYDROGENS allows the user to remove all hydrogen atoms from the current structure file, without changing the MM2 atom type of the (remaining) heavy atoms.

3.2.4 STRETCH

STRETCH allows the user to alter the scaling of the coordinate axes of a structure file. This can be useful in checking whether a the geometry represents a global or local minimum, providing a means of expanding or contracting the structure to check the optimization behavior. The user is prompted:

Enter Multiplication Factors <x,y,z>:

which expects the three factors (with decimal points) separated by commas. Numbers larger than one will increase the size and numbers smaller than one will decrease the size of the structure. Care must be taken to maintain some consistency of the coordinate axes when using this command.

3.2.5 CENCON

CENCON allows the user to translate the structure such that its center of charge, defined as a geometric average of the coordinates, weighted by atomic number, lies at the origin. This is useful in centering a structure for display purposes, or after molecular fragments have been added or deleted.

3.2.6 PRINAX

PRINAX allows the user to rotate the structure such that the principle atomic number moments are oriented along the cartesian axes, with the axis of highest principle moment

corresponding to the x-axis.

3.3 Structure Maintenance

These commands allow the user to obtain information on the run-time and revision status of MMADS, tailor the execution parameters to provide a more suitable working environment, perform interrogation and preparation operations on structure files and maintain the set of equilibrium values and force constants needed for molecular mechanics calculations. In addition, routines exist to transform structure files from MMADS internal format to that acceptable to other molecular modeling packages.

3.3.1 ENABLE/DISABLE

This pair of commands enable the user to alter flags which govern the operation of MMADS. The ENABLE command instructs MMADS to perform the action and the DISABLE command instructs MMADS to not perform the actions listed below. The default value for each option is provided in the option's description.

BATCH LOGGING When ENABLEd, all batch job log files will be retained. When DISABLEd (default), all batch job log files will be deleted.

CUSTOMIZATION When ENABLEd, MMADS looks in the current directory for the user's Customization file. When DISABLEd (default), MMADS ignores Customization files. This facility (described in Appendix XXX) allows the user to add new commands and/or alter existing commands as needed.

KEEPING FILES When ENABLEd, MMADS will retain all intermediary files created during the course of a terminal session. When DISABLEd (default), MMADS deletes all intermediary files. Care should be taken when using this option, so as to avoid clogging a directory with unnecessary files.

ANSWER FILE When ENABLEd, MMADS will create an answer file when the MM2 command is used. When DISABLEd (default), no answer file is created. This file contains a detailed description of the energetics of the optimized structure, both as an aid to the user and as required information to other MMADS commands.

NOTIFICATION When ENABLEd, MMADS will notify the user upon completion of any batch job summitted from within MMADS. When DISABLEd (default), no notification is given.

3.3.2 WHERE

WHERE indicates the current (sub)directory (in case the user forgets).

3.3.3 NEWS

NEWS displays the revision history of MMADS for the user, providing a means of reviewing the changes that have been made to the system. As MMADS is an evolving system, this command is useful in judging the degree to which the system has changed since the user last used it. New features are indicated in the news file as well, giving a better description than is possible in the introductory notes. The command pauses every twenty lines (permitting the user time to read), prompting the user to continue.

3.3.4 COMMANDS

COMMANDS lists the MMADS commands currently available to the user. The user is reminded that each can be abbreviated, and upper or lower case characters can be used throughout MMADS.

3.3.5 FILES

FILES lists the structure files, along with their version numbers, contained in the current (sub)directory.

3.3.6 PARAM

PARAM allows the user to specify the parameter file that will be used with subsequent MM2 optimizations. The user is prompted:

Enter parameter file name [(current file)]:

where (current file) is the name of the current MM2 parameter file. The parameter file is not changed if the user enters a blank line, and MMADS assumes that the default file (TRB$LIBRARY:BUD.PRM) will be used unless specified otherwise. All parameter files are maintained via BUDEDIT.

3.3.7 COMMENT

As MMADS is a developing system, suggestions for improvements, along with reports of bugs are greatly appreciated. This command allows the user to send mail to the developers, providing a hard copy of any comments. The user is directed to the NEWS file, the introductory comments or the VAX/VMS MAIL utility when looking for a response.

3.3.8 KEYPAD

KEYPAD allows the user to change the operation of MMADS to permit a user interface based on the terminal's keypad. When KEYPAD is enabled, commands not included on the keypad can be entered at the MMADS prompt. In KEYPAD mode, MMADS pauses after each command before (re)displaying the keypad commands.

3.3.9 EXIT

This command exits from MMADS, returning the user to the VAX/VMS operating system.

3.3.10 HELP

This command allows the user to obtain help on the operation of MMADS, invoking the VAX/VMS Help librarian (as if the user typed HELP MMADS to the DCL prompt).

3.3.11 CONMERGE

CONMERGE allows the user to merge a collection of structure files, while enforcing a specific orientation and coordinate system. CONMERGE prompts the user for several pieces of information:

Enter output structure name:

which expects the name of the (merged) structure file to be created,

Enter input structure name:

which expects the name of an existing structure file,

Enter origin atom:

which expects the index of the atom to be translated to the origin of the new coordinate system,

Enter atom defining first axis:

which expects the index of the atom defining the first axis of the new coordinate system,

Axis is (x=1, y=2, z=3):

which expects the cartesian axis corresponding to the first axis,

Enter atom defining the second axis:

which expects the index of the atom defining the perpendicular to the first axis, and

Axis is (x=1, y=2, z=3):

which expects the cartesian axis corresponding to the second axis.

This process is repeated for each additional structure file, until the user enters a blank line for the input structure name.

3.3.12 CONBREAK

CONBREAK allows the user to separate the molecules contained in a merged structure file into individual files. CONBREAK renumbers the atom indices, preserving the orientation and coordinate system in the individual structure files. CONBREAK prompts the user for several pieces of information:

STRUCTURE NAME =

which expects the name of the merged structure file. Once the file is read, the user is provided with a short description of its contents. For each structure found in the merged file, the user is prompted:

NEW STRUCTURE NAME -

which expects the name of the structure file to be created, and

ENTER 50 CHAR. OF IDENTIFICATION

which allows the user to specify the title of the new structure file. Once all new structure files have been created, the user is prompted:

BREAK-UP ANOTHER FILE (Y OR N)? [N]

If so directed, CONBREAK proceeds as if the user reentered the command at the MMADS prompt.

3.3.13 EMPIRICAL

EMPIRICAL allows the user to obtain the molecular and empirical formulae for a structure file. The molecular formula is a simple count of the individual atoms in the structure (by type), and the empirical formula is the count after all common divisors have been removed.

3.3.14 BBD

BBD allows the user to examine the nearest-neighbor bond lengths, angles and dihedrals of a structure, producing a listing on the VAX printer. Atoms are defined as nearest-neighbors if the distance separating them is within 120_% of the sum of their respective contact radii. Only parameters containing atoms meeting this criterion will be listed. If KEEPING FILES is ENABLEd, the output from BBD is written to disk (file suffix _.BBD) rather than being sent to the printer.

3.3.15 NEAREST

NEAREST allows the user to alter the connectivity of a structure file to reflect nearest-neighbor bonding. This has two possible applications: generation of a rough bonding environment for a structure file entered as atomic coordinates (e.g., via CRYSTAL) or as a means to rationalize the bonding environment after a geometry optimization. NEAREST prompts the user:

Enter nearest-neighbor factor [1.2]:

allowing the user to specify the multiplication factor to be applied to the contact radii used to determine whether two atoms are nearest-neighbors.

3.3.16 DATCON

DATCON allows the user to convert a structure file into the format acceptable to CHEMLAB or recover a CHEMLAB file for use with MMADS. The user is prompted:

Enter (full) filename to convert:

Which expects the name of the structure file to convert. DATCON uses the file suffix (see Appendix II) to determine whether the output is to be a MMADS or a CHEMLAB structure file. The number of atoms is provided, as a check for the user, along with any information on invalid or unsupported atom types.

3.3.17 TRIQUI

TRIQUI allows the user to convert a structure file into the format acceptable to QUIPU or recover a QUIPU file for use with MMADS. The user is prompted:

Is the target package Quipu(Q) or MMADS(M):

which expects the name of the system the structure file is intended for, and

Enter the filename:

which expects the name of the structure file to convert. No file suffix is required by TRIQUI. The user is notified if the conversion was successful, or if any errors were encountered.

3.3.18 ZCON

ZCON allows the user to convert structures defined by a z-matrix, as used by the ab initio quantum programs Gaussian-80 (UCSF) or Gaussian-82, into a structure file. ZCON accepts extracted z-matrices from both Gaussian-80 (UCSF) and Gaussian-82 output files, along with input files used by Gaussian-80 (UCSF). In addition, when processing output from Gaussian-80 (UCSF), ZCON can generate a replacement z-matrix that can be used to (re)create an input file. As with the structure files created by CRYSTAL, all atom types and connectivities must be supplied by the user. ZCON prompts the user for several pieces of information:

Is this a G80 or G82 file [G80]:

which allows the user to specify the particular ab initio program being used,

Enter input filename:

which expects the name of the input file to use. If the user has specified G82 as the file type, the file must be an extracted z-matrix with the suffix _.TMP. If the user has specified G80 as the file type, ZCON prompts:

Is this an extracted file (Y/N) [Y]:

which allows the user to specify whether the input file is an extracted z-matrix (file suffix _.TMP) or an input file (file suffix _.DAT). If an extracted z-matrix is being processed,

ZCON prompts:

Create replacement file (Y/N) [N]:

which allows the user to specify whether a replacement file should be created. This file, with the suffix _.INS, can be used to (re)create an input file for Gaussian-80 (UCSF).

3.3.19 ZTRANSLATE

ZTRANSLATE allows the user to extract a z-matrix from a Gaussian-80 (UCSF) output file, and create a new file (file suffix _.DAT) suitable for (re)input into Gaussian-80 (UCSF). ZTRANSLATE informs the user as to the number of z-matrices found in the Gaussian-80 (UCSF) output file, and prompts:

Use which version [<last>]:

which allows the user to specify which version of the z-matrix will be extracted.

3.3.20 MOPCON

MOPCON allows the user to convert the output and archive file created by the semi-empirical quantum program MOPAC after a successful optimization into a structure file suitable for use with MMADS. MOPCON performs all operations using the current structure name. The atom types are estimated, and MOPCON assumes that all "nearest-neighbor" atoms are bound. MOPCON prompts the user for several pieces of information:

MOPAC 2 or MOPAC 3 [3]:

which expects the version of MOPAC used to create the output files and

Recover structure version number [2]:

which expects positioning information on the particular z-matrix to extract as the output structure file. This is particularly useful when using MOPAC to study the reaction coordinate of a molecule.

3.3.21 INTERNAL

INTERNAL allows the user to generate an initial z-matrix for use by Gaussian-80 (UCSF), Gaussian-82 or MOPAC. Using tabulated nearest-neighbor parameters, INTERNAL generates an file with the suffix .INT that can be included in a data file of a future calculation. The user is cautioned that the output file is NOT guaranteed to be

entirely correct, as INTERNAL includes a zero value for z-matrix elements that are indeterminate. INTERNAL prompts the user for several pieces of information:

Enter nearest-neighbor factor [1.2]:

which expects the nearest-neighbor factor for use in determining the bonding in the current structure and

Enter output file type (G80, G82, MOPAC) [G80]:

which allows the user to specify the format of the output file. When the output file is in Gaussian-82 format, INTERNAL provides a rough guess of the geometry variables that might be used to define the z-matrix.

9.3.22 BUDEDIT

BUDEDIT is the MM2 parameter file editor. Using BUDEDIT, the user can maintain individual parameter files, thus tailoring MM2 to specific projects or molecules. While the VAX/VMS editor can be used for maintaining such files, BUDEDIT preserves the internal information needed to retain compatibility with MM2. Once entered, BUDEDIT prompts the user:

BUD> PARAMETER FILE NAME =

which expects the name of the parameter file to use. BUDEDIT accepts the following commands:

ADD	Add an entry to the parameter file. This entry MUST be unique.
EDIT	View, edit or delete an existing parameter. The user will be informed if the specified parameter is unknown.
QUIT	Exit BUDEDIT without saving the current information. This allows the user to perform editing operations without endangering the contents of the parameter file.
EXIT	Exit BUDEDIT normally, saving the current information. The input parameter file is rewritten upon program termination.

When ADD or EDIT is issued for the first time, the user is prompted for the comment to be attached to all changes or additions generated during the current BUDEDIT session. In addition, ADD and EDIT accept the following subcommands:

BEND Add or edit a bending parameter.

STRETCH Add or edit a stretching parameter.

TORSIONAL Add or edit a torsional parameter.

EXIT Return to command mode.

3.3.23 USE/INCREMENT/PROCESS

MMADS provides the user with several methods for specifying the current structure name:

USE <name> Set the current structure name to <name>.

If the structure name is omitted, MMADS prompts the user;

Structure name [<name>]:

where <name> is the current structure name. If the specified structure file does not exist in the current directory, the user is informed that it is a new structure file. The user can still enter a blank line at the MMADS prompt, as this archaic form is still supported (acting as the use command).

INCREMENT i Add the specified increment to the current structure name. If i is omitted, it is assumed to be 1. In order to use this command, the structure file must end in a number.

PROCESS i Set the numeric suffix of the current structure name to i. If i is omitted, the user is informed of the error. In order to use this command, the structure file must end in a number.

3.3.24 DEVICE

The display commands in MMADS direct their output to the current graphics device. The DEVICE command allows the user to specify the current device, prompting:

Enter terminal type (4010,4105,VT100,GPX):

where 4010 and 4105 are Tektronix monochrome and color terminals, VT100 indicates a terminal with no graphics capabilities and GPX is the DEC uVAX-II/GPX. MMADS does not assume a default graphics device.

3.3.25 BELL

BELL rings the bell on the user's terminal. This is designed to be included into MMADS script files as a means of catching the user's attention.

3.3.26 SCRIPT

SCRIPT allows the user to create a script file, a file containing a sequence of MMADS commands that can be applied to a list of structure files. SCRIPT prompts the user:

Enter script filename:

which expects the name of the script file to be created, and

Command:

which expects a valid MMADS command. The user is informed if the specified command is invalid, and SCRIPT prompts for additional commands until the user enters a blank line. The script file has a suffix of _.SCP.

3.3.27 EXECUTE

EXECUTE allows the user to apply an existing script file to a list of structure files. The format of the EXECUTE command is:

EXECUTE <script> <file1>,<file2>,...,<filen>,

where <script> is the name of the script file to process, and <file1>, <file2>, ... <filen> are the names of the structure files to use. If the user neglects to specify the script name, EXECUTE prompts:

Enter script filename:

which expects the name of an existing script file. If the user neglects to specify any structure files, EXECUTE prompts:

Enter structure files:

which expects a list of structure files separated by commas. EXECUTE informs the user that the script is being started, the particular structure file being processed and that the script has terminated. If the user specifies a non-existant structure file, EXECUTE indicates the error.

3.3.28 MIRROR

MIRROR allows the user to reflect a structure about any of the Cartesian coordinate axes. MIRROR prompts the user:

Enter coordinate axis (x,y,z):

which expects the coordinate axis to use as the mirror plane. For example, if the x-axis is specified, the coordinates of each atom in the current structure file will be transformed (xi,yi,zi) --> (-xi,yi,zi).

3.3.29 STATUS

STATUS allows the user to query MMADS for several pieces of information: the current structure name, the current (sub)directory, the current MM2 parameter file, the current graphics device and whether MMADS has been customized. In addition, if any of the flags specified by the ENABLE/DISABLE commands have been changed, the user is informed of their current value.

3.3.30 WEIGHT

WEIGHT allows the user to obtain the molecular weight of the current structure. For correct operation, the MM2 atom type of each atom in the structure file must be specified.

3.3.31 RESET (CBM VAX-11/730 Only)

RESET allows the user to reset the Adage 3000 Raster Display System to ensure that the SPHERE command will work properly.

3.3.32 XYZ

XYZ allows the user to generate an initial cartesian representation for use by MOPAC, reformatting the information contained in a structure file into a suitable form. XYZ prompts the user:

Create a MOPAC input file (Y/N) [Y]:

which allows the user to specify whether a MOPAC input file (file suffix .MNI) or an

intermediate file (file suffix _.XYZ) should be created.

3.3.33 SURROUND

SURROUND allows the user to surround a molecule with an arbitrary number of randomly oriented water molecules, at an arbitrary minimum and maximum distance from its Van der Waals surface. SURROUND centers the current structure at the origin, and prompts the user:

Number of water molecules to generate [6]:

which expects the number of water molecules to be added, and

Enter minimum,maximum water distances [3.0,6.0]:

which expects the minimum and maximum distance (in Angstroms) from the Van der Waals surface a water molecule can be located. Finally, SURROUND prompts:

Enter title line:

which allows the user to specify the title of the (new) structure file. SURROUND uses the current structure file name when creating its output file.

3.3.34 WATER_SHELL

WATER_SHELL allows the user to surround a molecule with 14 water molecules located at the vertices and the center of each face of a rectangular prism containing the current structure, located at an arbitrary distance from its Van der Waals surface. WATER_SHELL prompts the user:

Enter the water shell size (3 Angstroms suggested):

which expects the approximate distance between the Van der Waals surface and the rectangular prism, and

ZINDO optimized, MOPAC optimized or EXP H2O structure:

which allows the user to specify which geometry for the water molecules will be used. WATER_SHELL informs the user that a new version of the current structure file (as with SURROUND) has been created.

3.3.35 CONNECT

CONNECT allows the user to alter the connectivity and atom types of a structure file to conform to the bond order information provided by MOPAC. This information is included in the MOPAC output file (file suffix _.MNO) when the BONDS option is invoked. To ensure proper results, MOPCON must be used to create a structure file before using CONNECT.

3.4 Structure Optimization

These commands allow the user to optimize the geometry of a structure, through minimization of the molecular potential function. Five models are currently available: three are "true" Molecular Mechanics algorithms and two use a simple harmonic representation of the molecular potential function. All of the Molecular Mechanics routines use the Allinger MM2 force field. In cases where geometric parameters are unavailable, a modified Allinger MM2, treating all atoms as carbons and hydrogens, is available.

Owing to programming limitations, the programs based on the Allinger force field are limited to structures containing five hundred (BS3, one hundred) or fewer atoms. The harmonic models can be used as a means of obtaining optimized structures when larger molecules are involved. Due to the simplicity of their force fields, a considerable reduction in computational intensity is obtained by their use.

3.4.1 MM2

The Allinger force field views a molecule as made up of a collection of harmonic bond lengths and angles, cyclic torsional angles, twisting modes (based on simultaneous bond stretch/bend), 1-4 interactions and electronic interactions. Using a list of these parameters (either experimentally or theoretically determined), MM2 attempts to produce a geometry that conforms as closely as possible to these standard values.

This technique has two limitations. As the force field was developed for standard organic chemistry, it is somewhat incomplete in its treatment of the atoms that are important to inorganic chemistry (and are larger than flourine). These missing parameters are beind determined from ab initio quantum chemical calculations (at the 4-31G* level). In addition, the maximum number of atoms that can be dealt with using MM2 is 500. In spite of these limitations, MM2 remains an extremely useful tool.

MM2 prompts the user for several pieces of information:

Initial energy only [N]:

which allows the user to specify that no minimization is to be performed. In such cases, MM2 will evaluate the steric energy of the current structure without altering it through optimization. If geometric parameters required by any calculation are unavailable, an estimate of the initial energy is provided before MM2 terminates.

Enter CPU time limit [5]:

which expects the time limit, in minutes, for the optimization.

Program Output

1. MM2 provides information of the average atomic displacement with each iteration. In addition, the energy terms of the potential function are provided every five iterations. The molecular geometry and the final value of the energy terms are provided on completion.

2. When a calculation results in an optimized structure, an extensive description of the steric energy of each geometric parameter of the structure is provided if ANSWER FILES is ENABLEd. This answer file is saved in the current (sub)directory with the file suffix _.MM2.

3.4.2 CRUDE

CRUDE allows the user to use the Allinger force field to optimize structures that require parameters that are currently unavailable. All heavy atoms are treated as carbons, with all other atoms treated as hydrogens. This modified structure is then optimized.

Several differences with MM2 must be noted: CRUDE only prompts the user for the CPU time limit for the calculation and no answer file can be produced. The initial and final geometries are displayed on the user's terminal, along with the iteration by iteration information previously described. Care must be taken when optimizing structures with CRUDE on account of the approximate nature of the result(s).

3.4.3 CPK

This command allows the user to optimize the geometry of a structure file using a simple, idealized potential energy function. Bonds are represented as a harmonic stretching term, while non-bonded (collision only) interactions are represented as a gaussian interaction term. The optimized geometry is produced by minimizing the the resulting energy function.

With each iteration, CPK indicates the current value of the energy function, along with the rms change in the value of the function since the last iteration. Minimization is terminated when fifty iterations have been completed, or when the rms change is less than 0.001. If the iteration limit is reached, additional CPK optimizations should lead to an optimized structure.

One major problem has been noticed in the operation of CPK - it is unable to "break" the initial symmetry of the molecule. For example, if all atoms of a structure lie in the x-y plane, all atoms in the optimized structure remain in that plane. This can result in structures having hydrogens located at the same coordinates, since CPK is unable to use the (missing) z-coordinate to separate them. The maximum number of atoms that can be dealt with using CPK is 200.

3.4.4 MODEL

MODEL allows the user to optimize the geometry of a structure file using a potential energy function qualitatively similar to that used by CPK. MODEL provides the user with several improvements: First, the bond stretching and atom collision terms are parameterized for all atoms in the periodic table. Second, the user can alter the coefficients associated with each term in the potential energy function. Finally, MODEL provides the user with a graphical display of the molecular structure as the optimization progresses.

The user is prompted:

Structure file in standard format (Y/N) [Y]:

which allows the user to specify whether the atom types in the structure file are correct. If the atoms are properly typed, MODEL uses this information to improve its treatment of multiple bonds.

Model accepts the following commands:

Potential Energy Function

ALPHA x Change the strength of the non-bonded interaction term (ALPHA*exp(-rij/beta) to x.

BETA x Change the range of the non-bonded interaction term (alpha*exp(-rij/BETA) to x.

GAMMA x Change the strength of the bonded interaction term (0.5*GAMMA*(rij-ideal)**2) to x.

Display options

XROT x Rotate the display x degrees about the x-axis.

YROT x Rotate the display x degrees about the y-axis.

ZROT x Rotate the display x degrees about the z-axis.

where the screen is the x-y plane, and +z extends towards the user.

Structure Optimization

RMIN x Change the convergence criterion to x. Minimization will cease when the change between successive iterations is less than this value.

RMAX x Change the maximum atomic displacement that can occur on a single iteration to x. Care must be taken when increasing this value to any great degree as the resulting calculations can become divergent.

ITERATE Perform x minimization iterations. The structure is displayed every ten iterations, with the screen redrawn every thirty iterations.

QUIT Exit MODEL without saving the current structure.

EXIT Exit MODEL normally, saving the current coordinates.

HELP Obtain help on the operation of MODEL.

All parameters included with MODEL commands must be real numbers. Invalid commands, or commands with improper parameters will be ignored without altering the display.

3.4.5 BS3

BS3 allows the user to optimize the geometry of a structure file using the Allinger MM2 force field and geometric parameters as implimented in the Bigstrain-3 molecular mechanics program developed at Merck and available from QCPE. Due to the limitations of the interface between MMADS and Bigstrain-3, the three alternative molecular mechanics force fields included in the QCPE distribution are unaccessable (although they are included for possible future use). The user is referred to the Bigstrain-3 documentation if additional information is desired.

As currently implemented, BS3 optimizes the molecular geometry using a Newton-Raphson (second order) minimization procedure. While the geometric parameter set is incomplete, BS3 can be used with the structures encountered in "traditional" organic chemistry. It requires a partial structure file (described below) as a starting point, producing a optimized structure file if the minimization is successfully completed. The maximum number of atoms that can be dealt with using BS3 is 100.

KWIKDRAW must be used to create the partial structure file required by BS3, with one significant exception: the user MUST specify that hydrogen atom generation is to be suppressed. BS3 will generate whatever hydrogens are necessary to fill the valence shell of each atom in the structure file, including them in the optimized structure file (if created).

BS3 prompts the user for several pieces of information:

Time limit for minimization (min) [10]:

which expects the CPU time limit for the optimization, and

Interactive, Batch, Fast or Defer [Batch]:

which allows the user to specify whether the optimization is to be performed at the user's terminal, submitted to the system batch or fast batch queue or deferred. If the optimization is successful, BS3 prompts the user:

Make corrections to the structure file (Y/N) [Y]:

which allows the user to specify whether an optimized structure file should be created. If BS3 is run from a batch queue, an optimized structure file will be created.

BS3 creates an output file (file suffix _.BOU) that contains an extensive description of the minimization process. If the optimization is successful, BS3 creates a summary file (file suffix _.BS3) that contains the optimized geometry in a form suitable for input into additional BS3 calculations.

3.4.6 TMODELER

TMODELER is MODEL Version 1.3, integrated into MMADS. Due to programming limitations within MODEL, the only supported graphics device is the Tektronix 4010 (monochrome) terminal. TMODELER supports an elegant mouse-driven interface,

allowing the user to easily create, edit, optimize and view (including stereo projection) structure files. The user is referred to the MODEL documentation for additional information on the operation of TMODELER.

3.5 Property Determination

These commands allow the user to determine steric and electronic properties of a structure, without altering the molecular geometry. Four physical properties can be calculated: the molecular surface area, the molecular volume, the volume shared between two molecules and the solvent-accessible surface area. One electronic property can be calculated: the electrostatic potential based on an INDO/S wavefunction. Several other descriptors are under development and are contained in the EIGEN and VECTOR commands.

3.5.1 AREA

AREA calculates the total surface area of a molecule. This is determined using a summation of the exposed surface area of each atom, represented as a sphere with the appropriate Van der Waals radius. An estimation of the area of the structure/solvent aggregate can be obtained as well. The user is prompted:

Enter solvent radius [0.0]:

which expects the radius of the solvent molecules. This value is added to each Van der Waals radius before determining the area. AREA lists each atom in turn, indicating the atom symbol and the percentage of the surface that is exposed, along with the final value of the surface area (in A^2).

3.5.2 VOLUME

VOLUME calculates the total volume occupied by a molecule. This is determined using a summation of the volume of each atom, represented as a sphere with the appropriate Van der Waals radius, taking care to avoid overcounting shared volumes. The user is prompted:

Enter x-increment [0.1]:

and

Enter z-increment [0.1]:

These two parameters determine the resolution of the numerical integration grid used to

calculate the molecular volume, and thus the degree of computational intensity required. Care must be taken when comparing volumes obtained with different values of these parameters.

3.5.3 MSA

Molecular Shape Analysis (MSA) determines the total volume shared between two molecules. This is useful in evaluating the degree of similarity between molecules sharing a common orientation and coordinate system. MSA does not change the contents of any of the structure files involved. The user is prompted:

Enter second structure:

which expects the name of an existing structure file,

Enter x/z-increments [0.1]:

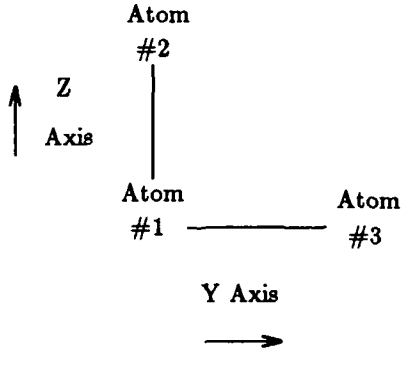
as with VOLUME,

Enter the three atoms of molecule _#1:

which expects the atom triplet of molecule _#1 to use,

Enter the three atoms of molecule _#2:

which expects the atom triplet for molecule _#2. These last two prompts allow the molecules to be properly oriented, using the following coordinate system:



For both molecules, the first atom of the triplet is translated to the origin. The second atom is aligned with the cartesian z-axis and the third is aligned with the cartesian y-axis.

MSA provides three molecular volumes to the user: the volume of each individual structure and the overlap (or shared) volume using this particular configuration. The user is reminded that the overlap volume is totally dependent on the proper alignment of the individual structures. The use of arbitrary configurations guarantee that the overlap volume determined is irrelevant.

3.5.4 MVOLUME

MVOLUME allows the user to determine the molecular volume using a Monte Carlo approximation to the numerical integration employed by VOLUME. If the structure is assumed to lie in a box slightly larger than the maximum displacement along each coordinate axis, the volume is defined as:

$$V_m = f*V_b$$

where V_b is the volume of the box, f is the fraction of the randomly located points that occur within the Van der Waals radius of any atom and Vm is the (resulting) molecular volume (in A^3). MVOLUME prompts the user:

Enter the number of points to use [30000]:

which expects the number of points to be used in the approximation. Increasing the number of points will improve the accuracy of the calculation, as well as increase the computational intensity that is required. As the time required to determine the volume is dependent on the number of points generated. MVOLUME might have some use when investigating very large structures.

3.5.5 GVOLUME

GVOLUME allows the user to determine the molecular volume using a numerical integration in three dimensional Cartesian coordinate space. If the structure is assumed to lie in a box slightly larger than the maximum displacement along each coordinate axis, the volume is defined as:

$$V_g = f*V_b$$

where Vb is the volume of the box, f is the fraction of the grid points that occur within the Van der Waals radius of any atom and Vg is the (resulting) molecular volume (in A_^3).

GVOLUME prompts the user:

Enter grid increment [0.25]:

which expects the value (in Angstroms) to be used as the step size along each axis when constructing the 3-D grid. Increasing the number of points will improve the accuracy of the calculation, as well as (dramatically) increase the computational intensity that is required.

3.5.6 SHARED

SHARED allows the user to determine the molecular volume shared between two molecules using a Monte Carlo approximation (see MVOLUME) to the numerical integration employed by MSA. The user is prompted:

Enter second structure:

which expects the name of an existing structure file,

Enter the three atoms of molecule _#1:

which expects the atom triplet of molecule _#1 to use,

Enter the three atoms of molecule _#2:

which expects the atom triplet for molecule _#2. SHARED uses the same orientation scheme used in MSA.

Enter the number of points to use [30000]:

as with MVOLUME. MVOLUME provides the user with the same information provided by MSA.

3.5.7 CONOLLY

CONOLLY allows the user to investigate the solvent-accessible surface of a structure. The solvent-accessible surface is (briefly) defined as that surface which is a) in contact with a solvent molecule or b) formed by the inner surface of a solvent molecule resting in a cavity on the molecular surface. Solvent molecules are modeled as spheres of a user-

specified radius.

The first surface, consisting of all points that are tangent to both a solvent molecule and an atom of the structure, is defined as the contact surface. The second surface is defined as the reentrant surface, and can only be generated when using real (i.e. radius >#0.0) solvent particles. The Van der Waals surface is produced if a solvent radius of zero is used.

CONOLLY consists of three parts: surface generation, determination of the electrostatic potential and the display utility. The following commands are available:

CALCULATE	Generate the solvent-accessible surface.
ELESTA	Calculate the values of the electrostatic potential (using the INDO/S Hamiltonian) at each point of the surface.
PLOT	Display the surface, color-coded by atom type, formal charge or electrostatic potential.
EXIT	Exit Conolly.
HELP	Obtain help on the operation of CONOLLY.

Surface Generation

CALCULATE allows the user to generate the solvent-accessible surface. This creates the surface file(s) that are required for proper execution of the ELESTA and PLOT subcommands. The user is prompted:

Enter _#points/area [6]:

which expects the number of points to calculate per unit area,

Enter solvent radius [0.0]:

which expects the solvent radius. If a blank line is entered, only contact surface is determined.

At this point, CONOLLY determines the desired surface. Several pieces of information are provided for the user: the number of atoms involved, the number of points in the

display, the total contact area, the total reentrant area and the total surface area. For the display routine to function properly, the number of points generated must be 30,000 or fewer.

Calculation of the Electrostatic Potential

ELESTA allows the user to determine the value of the electrostatic potential at each of the points contained in the surface file generated by CALCULATE. In addition, the user can specify a scaling factor to examine surfaces different than the actual solvent-accessible surface. Before ELESTA can be invoked, a stationary ZINDO calculation must be carried out (to obtain the density matrix and wavefunction). The user is prompted:

Enter scaling factor for elesta plot [1.0]:

which expects the scaling factor to be used. The length of the vector from the center of mass to each individual surface point is multiplied by this factor. Suggested values for the multiplication factor are in the range of 1.5 to 2.5.

Surface Display

PLOT allows the user to view the solvent-accessible surface on a graphics device as an array of points drawn over a color-coded stick-figure representation of the molecular geometry (see STICK). Currently, PLOT supports four color-coding schemes: by nearest atom, by formal charge, by electrostatic potential and by x-coordinate (a debugging tool).

The display routine accepts the following commands:

XROT x	Rotate the surface x degrees about the x-axis.
YROT x	Rotate the surface x degrees about the y-axis.
ZROT x	Rotate the surface x degrees about the z-axis.
PLOT	Display the surface, using the current orientation.
DISPLAY	Indicate the current display option.
DISPLAY CONTACT	Display the contact surface only.
DISPLAY REENTRANT	Display the reentrant surface only.

DISPLAY BOTH	Display the entire surface.
COLOR	Indicate the color scheme in use.
COLOR PLOT	Color points by nearest atom.
COLOR ELESTA	Color points by the value of the electrostatic potential at each point.
COLOR ZERO	Color points by the value of the electrostatic potential estimated from the formal charges at each point.
COLOR FORMAL	Color points by the formal charge of the nearest atom.
COLOR XSCALE	Color point by their x-coordinate in the display (debugging tool).
STYLE	Indicate the display style in use.
STYLE LIGHT	Perform light hidden-point removal.
STYLE RIGOROUS	Perform rigorous hidden-point removal.
STYLE DRAW	Include a stick figure in the display.
STYLE OMIT	Omit the stick figure from the display.
RADIUS x	Set the radius used to determine hidden points to x Angstroms.
SCALE x	Set the scaling factor used to color points by electrostatic potential to x au.
EXIT	Exit the DISPLAY Submode.

All rotation angles must be be entered in degrees. Invalid commands or commands with improper parameters will be ignored without altering the display.

3.5.8 CONE

CONE allows the user to determine the Tolmann cone angle for substituent groups coordinated with a metal ion. In addition, CONE allows the user to view the molecular geometry and bonding environment of individual atoms in the current structure file, as well as review the Van der Waals radii currently in use. The user is directed to the journal article Chem. Rev. ^&77, 313(1977) for additional details on the development and use of this descriptor. CONE accepts the following commands:

VIEW <atoms>	Display the atom symbol, index, coordinates, type and connectivity of the specified atoms.
LIST	Display the above information for the entire molecule. The display pauses every 20 atoms, prompting the user to continue.
ANGLE	Indicate the Tolman cone angle between the specified atoms. CONE assumes that the central atom is the metal atom.
VLIST	Display the value of the Van der Waals radius associated with each MM2 atom type supported by CONE.
EXIT	Exit CONE.
HELP	Obtain help on the operation of CONE.

The VIEW command uses the free-format input described previously. If the parameter <atoms> is omitted, the user will be prompted for the atoms to be viewed. When executing commands in this manner, only one atom can be dealt with at a time. For all commands, incorrect values, or references to missing atoms will be reported.

3.5.9 ELESTA

ELESTA allows the user to calculate the electrostatic potential surrounding the current structure at each point of a three dimensional grid in Cartesian coordinate space, using the INDO/S Hamiltonian. ELESTA assumes that the density matrix and molecular wavefunction has been created using ZINDO, and creates a file (file suffix _.ELS) containing the values of the electronstatic potential for use by C3D. ELESTA prompts the user:

Enter contour value [0.05]:

which expects the value of isopotential surface to generate. This request is required to support several archaic commands present in earlier versions of MMADS, and can be basically ignored by the user. Next, ELESTA prompts:

Interactive, Batch, Fast or Defer [Batch]:

which allows the user to specify whether the calculation is to be performed at the user's terminal, submitted to the system batch or fast batch queue or deferred. The user is strongly encouraged to perform all ELESTA calculations in the background, on account of the large amount of computational effort required.

3.5.10 EIGEN/VECTOR

These two commands are highly experimental, generating several steric (EIGEN) and/or electronic (VECTOR) descriptors for the current structure file. Before VECTOR can be used, a formal charge file must have been created using ZINDO or MOPAC/MOPCON. EIGEN can also be used to orient a structure file along the principle components of the molecular coordinates. These two commands represent unpublished, and generally unproven algorithms, which might be useful. If additional information is required, the user should contact the author.

3.5.11 HYDRATE

HYDRATE allows the user to determine the distance separating each water molecule from the hydrated molecule in a structure created by SURROUND or WATER_SHELL. Three distinct distances can be calculated: from the Van der Waals surface, from the center of mass or from a particular atom in the hydrated molecule. If KEEPING FILES is ENABLEd, the output from HYDRATE is written to disk (file suffix _.HYD) rather than being sent to the printer. HYDRATE indicates the total number of molecules found in the current structure file, and prompts the user:

Use VDW surface (V), atomic center (A) or center of mass (C) [V]:

which allows the user to indicate the particular distance algorithm to use. If the atomic center option is specified, HYDRATE prompts:

Enter the atom to use:

which expects the index of the particular atom in the hydrated molecule to use as the central point for the distance calculations.

Each distance algorithm has a unique output format:

Van der Waals — Indicate that the Van der Waals surface is being used, specify the type and location of each atom in each water molecule, along with the type and index of the closest atom in the hydrated molecule along with the distance from the Van der Waals surface.

Center of Mass — Indicate that the center of mass is being used, and specify its location. Specify the type and location of each atom in each water molecule, along with the distance from the center of mass.

Atomic Center — Indicate that an atomic center is being used, and specify its type, index and location. Specify the type and location of each atom in each water molecule, along with the distance from the specified atom.

As implemented, the output from HYDRATE is somewhat obscure - this is intentional, as the command is still in the development stage. It is not known at this time whether HYDRATE will generate the input data for another program yet to be specified or whether it will be merely rewritten to improve readability.

3.5.12 ELECTOP

ELECTOP calculates the topological electronic index (in charge/A^2) for the current structure. It assumes that a formal charge file has been created using ZINDO or MOPAC/MOPCON. The user is directed to the journal article *Chromatogr* **2**,19(1987) for additional details on the development and use of this descriptor.

3.6 Graphical Display

These commands allow the user to use the various graphic display devices available on the MMADS host to view the geometry of structures created via MMADS. With these commands, the user can obtain a rough geometry on a non-graphics terminal, obtain a Newman projection about any bond, obtain a colored stick-figure representation, view structures with the Cambridge Crystallographic Database program PLUTO and obtain real-time, three-dimensional representations on the CBM Adage 3000 graphics engine.

3.6.1 DRAW

DRAW allows the user to obtain a crude representation of the molecular geometry on any terminal. This command can display either the atom symbols or indices, being the functional equivalent of the ADRAW/NDRAW subcommands of KWIKDRAW. The user is prompted:

Use atom symbols (S) or indices (I) [S]:

which allows the user to specify the symbols to be used. DRAW can be used to display structures containing one hundred or fewer atoms. The user is cautioned that the output from DRAW may be less than useful when the atom count is larger than fifty.

3.6.2 NEWMAN

NEWMAN allows the user to obtain a Newman projection along any bond in the current structure file. A graphics device is required for proper execution of this command. The user is prompted:

Enter rear atom index:

and

Enter front atom index:

NEWMAN expects these two atoms to be present in the structure and bound to each other. After the projection is drawn, NEWMAN requests additional atom pairs, terminating when a blank line is entered.

3.6.3 STICK

STICK provides many capabilities: (a) Structures can be viewed as a stick figure, "ball-and-stick" representation or contact-sphere representation ; (b) Color coding is used to describe the atom pair for each bond, as well as each atom in the "ball-and-stick" and contact-sphere representations; (c) Both orthographic and depth cued projections can be generated; (d) Atoms can be labeled by atom type or formal charge; (e) Individual atom types can be omitted from the display; (f) Up to ten structures can be simultaneously displayed; (g) Structures can be rotated about or translated along any of the Cartesian axes; (h) Structures can be saved to disk, scaled to a common coordinate system; (i) Bond Stretch/Bend and Torsional strain energies (as calculated by MM2) can be displayed, color-coded by magnitude; (j) Hydrogen bonds can be displayed, if the formal charges of each atom are known.

Currently, STICK supports the Tektronix 4010 and 4105 family of terminals, along with terminals (or software) that emulate either of these Tektronix terminals. In addition, STICK supports the Digital Equipment Corporation uVAX-II/GPX 2-D color graphics workstation. Future development will include support for the Adage 3000 raster graphics system and the Silicon Graphics IRIS color workstations. While this version of STICK is limited to static, two-dimensional displays, codes developed for the 3-D color workstations will provide additional capabilities, such as real-time animation.

STICK *Commands*

STICK commands can be broken down into four categories: plot format, plot content, plot orientation and general-purpose. Plot format commands allow the user to define the representation, select the color coding scheme, and indicate what (if any) atoms will be omitted from the display. Plot content commands allow the user to load, save and display multiple structures, and specify the labeling convention to be used in generating the

display. Plot orientation commands allow the user to rotate or translate individual structures (or the entire display), and change the scaling of the display. General-purpose commands allow the user to control the operation of STICK. The individual commands are described below, with verticals separating valid operands (if any) of each command.

Plot Format

STICK — This command instructs STICK to produce a "stick figure" representation for all structures loaded into the display. All bonds are indicated, color-coded by the atom pair making the bond. This is the default representation.

BSTICK — This command instructs STICK to produce a "ball and stick" representation for all structures loaded into the display. All bonds are indicated, and all atoms are color-coded by type.

SOLID — This command instructs STICK to produce a contact-sphere representation for all structures loaded into the display. All bonds are indicated, and all atoms are color-coded by type. In this representation, the "perfect" bond is represented by two circles tangent at one point.

STYLE STICKS | BOXES | <null>

This command instructs STICK to display all bonds as line segments (STICKS), or to represent all bonds as polygons, scaled to provide depth cueing (BOXES). If STYLE is entered without an operand, the current style is provided. The default style is STICKS.

OPTION COLOR | WHITE | OMIT | HBOND | NOHBOND | <null>

This command instructs STICK to color-code all bonds to reflect the atom pair (COLOR), color all bonds white (WHITE), omit all bonds from the display (OMIT), include (HBOND) or exclude (NOHBOND) hydrogen bonds from the display. If OPTION is entered without an operand, the current option is provided. The default options are COLOR and HBOND.

OMIT <atom1> ... <atomn> | <null>

This command instructs STICK to omit the specified atom types from the display. The OMIT command accepts multiple operands, and STICK accumulates the atom types for omission if several OMIT commands are issued. If OMIT is entered without an operand, the atom types that will be omitted are provided. Unless specified otherwise, all atoms are displayed.

STRAIN STRETCH | BEND | TORSIONAL | <null>

This command instructs STICK to color-code all bonds to reflect the bond stretch, bend or torsional energy associated with each internal coordinate of the molecule. This command requires information obtained from the MM2 answer file, and the user is informed if the data is unavailable. A spectral color-coding scheme is used to indicate energies in the range [0.0,4.0+] Kcal. If STRAIN is entered without an operand, the STRETCH option is assumed.

Plot Content

LOAD <filename>

This command loads the specified structure file into STICK, using the coordinates specified in the input file. If appropriate, the display is rescaled to contain the new structure. If more than one file has been loaded, STICK omits the title line of the display. The current structure (as defined when STICK is entered) is structure _#1, and STICK permits a maximum of 10 structures to be LOADed.

SAVE <number>,<filename> | <filename>

This command saves structure <number> in the specified structure file, using the current coordinate system of the display. If <number> is omitted, all structures are saved in the specified file. This option has turned out to be a useful side effect of STICK, providing a graphical means of merging chemical structures in a common coordinate system.

USE <number> | ALL | <null>

This command specifies that structure <number> is to be used by the rotation and translation commands, or that the entire display will be used. If USE is entered without an operand, the name and number of all structure files that have been LOADed are provided. Unless specified otherwise, structure _#1 is USEd.

VIEW <number> | <null>

This command toggles whether structure <number> will be visible or invisible on the display. If VIEW is entered without an operand, the view status of all structures is provided. Unless specified otherwise, all structures are visible.

LABEL LABELS | FORMAL | <null>

This command instructs STICK to label each atom in the display by its type and number (LABELS), or by its formal charge (FORMAL). On color terminals, the formal charge is color-coded by sign: magenta for positive values and red for negative values. For STICK and BSTICK representations, STICK endeavors to place the labels so they are not obscured by atoms in the display. For SOLID representations, the labels are placed at the center of each atom in the display.

THRESHOLD <value> | <null>

This command instructs STICK to omit the formal charge label for any atom with |FC| < <value>. Due to limitations of the graphics hardware, 0.01 is enforced as the minimum threshold value. If THRESHOLD is entered without an operand, the current value is provided.

Plot Orientation

XROT <value>

This command instructs STICK to rotate the current structure (as defined by the USE command) by <value> degrees about the x-axis.

YROT <value>

This command instructs STICK to rotate the current structure (as defined by the USE command) by <value> degrees about the y-axis.

ZROT <value>

This command instructs STICK to rotate the current structure (as defined by the USE command) by <value> degrees about the z-axis.

XTRANS <value>

This command instructs STICK to translate the current structure (as defined by the USE command) by <value> Angstroms along the x-axis. This command has no observable effect if the entire display is acted upon.

YTRANS <value>

This command instructs STICK to translate the current structure (as defined by the USE command) by <value> Angstroms along the y-axis. This command has no observable effect if the entire display is acted upon.

ZTRANS <value>

This command instructs STICK to translate the current structure (as defined by the USE command) by <value> Angstroms along the z-axis. This command has no observable effect if the entire display is acted upon.

SCALE + | - This command instructs STICK to increase the size of the display by 10% (+) or decrease the size of the display by 10% (-). Any alterations made via the SCALE command will be lost when rescaling is applied after a rotation or translation command is performed.

BLACK This command specifies that a dark background will be used in subsequent plots.

GREY This command specifies that a light background will be used in subsequent plots.

General-purpose

PLOT This command instructs STICK to generate a new display, using the various display parameters described in the previous commands.

RESET This command reinitializes STICK, as if the user exited and reentered the program. All parameters are restored to their default values, and all *LOADed structures are deleted.*

EXIT This command exits STICK.

3.6.4 PLUTO

PLUTO allows the user to display the configuration of a structure on a graphics device. The user can select a stick figure, ball and stick or solid (contact radii) representation, using parallel projection, perspective or stereo-pair projection. The view direction can be set with reference to molecular features such as lines and planes defined by individual atoms, or by reference to the cartesian axes. The view direction can be further modified by rotations about the plot reference axes.

PLUTO accepts the following commands:

The OPTION command

SOLID	Plot using covalent radii.
BSTICK	Plot using a ball and stick representation.
STEREO	Plot using stereo-pair projection.
NOLABEL	Suppress all atom labels.
NOHYD	Omit hydrogen atoms from the plot.
VIEWX	Set view direction along the cartesian x-axis.
VIEWY	Set view direction along the cartesian y-axis.
VIEWZ	Set view direction along the cartesian z-axis.

All the above suboptions can be entered as PLUTO commands as well. The OPTION command allows the user to specify several suboptions at the same time. If no options are specified, the following options are assumed: stick figure, single display with no perspective, no atom labels, include all hydrogen atoms and minimum overlap view direction set.

Display Generation

PERSP x	Projec 'he coordinates with perspective applied from a viewpoint x mm in front of the molecular plane. This is applicable to stereo-pairs as well.
SHADE x y	Define the shade lines representing shadow from a light source whose position is defined by the angles x and y. These are the angles from the Y and Z axis of the plot, respectively.
LABEL (list)	Label the atom types specified in (list). If (list) is omitted, label all atoms.
INCLUDE (list)	Plot (only) the atoms specified in (list).
EXCLUDE (list)	Exclude the atoms specified in (list) from the plot.

OMIT (list)	(as with EXCLUDE)
TITLE (title)	Change the plot title to that specified. (list) contains the atom symbols separated by spaces.

Display Alteration

RADII	Specify the radii of atom circles and bond cylinders and the number of lines used in drawing a bond. Used with the BSTICK and SOLID commands. Several options exist:
ATOMS (list)	Set the atom radii for the specified atoms to the values provided. (list) consists of pairs of atom labels and radii.
BONDS ALL x y	Plot all bonds with cylindrical radii of x Ang., drawing y lines per bond.
BONDS TO e x y	Plot all bonds to to atom type e with radii of x Ang, drawing y lines per bond.
BONDS TAPER x	Exaggerate the taper of individual bonds, thus enhancing the illusion of depth. Forty is a good upper limit for proper effect.
VIEW	Specify the (complex) view direction for the display. The initial plot attempts to display the largest number of distinct atoms. Five additional view directions are possible:
HOR a b VER c d	Define the plot x-axis as atom a –> b. Use the perpendicular most similar to atom c --> d as the plot y-axis.
LINE a b HOR c d	Define the view direction as a –> b. Define the plot x-axis as c –> d.
BISECT a b c	Define the view direction along the bisector of the angle a-b-c towards atom b.
PERP a b c	Define the view direction along the perpendicular of the plane defined by atoms a, b and c.
PLANE a b c d	Define the view direction normal to the plane defined by atoms a, b, c and d.

The view direction can be completely generalized, as PLUTO allows the user to take a defined orientation and rotate it successively about any of the plot axes:

XROT x Rotate x degrees about the plot x-axis.

YROT x Rotate x degrees about the plot y-axis.

ZROT x Rotate x degrees about the plot z-axis.

All of the options of VIEW can be combined in a single command. allowing the user to specify extremely elaborate orientations in a straightforward manner.

Other Commands

STICK Plot a stick figure, indicating atom connectivity.

PLOT Display the structure using the currently enabled display options.

SAVE Write the current orientation and connectivity into a structure file.

EXIT Exit PLUTO.

3.6.5 SPHERE (CBM VAX-11/730 only)

SPHERE allows the user to view structures in three dimensions, providing real-time rotation, translation and scaling capabilities. Two representations are available: spheres with Van der Waals or covalent radii. When displaying two structures, SPHERE allows the user to operate on individual molecules, or on the merged pair. Unlike other graphics routine in MMADS, SPHERE ignores the connectivity information contained in the structure file.

Using the Adage 3000 raster graphics engine, the user has full, continuous control of the display through the dialbox and joystick. The user is provided with a large set of keyboard options:

Input Device Assignment

d Set the Adage input device as the dialbox, and reset.

j Set the Adage input device as the joystick, and reset.

b Set both the dialbox and joystick as input devices. This is the default setting.

k Start the display rotating, using user-specified x, y and z rotation increments (in degrees).

a Describe the active Adage input device.

SPHERE assumes that both the dialbox and joystick are connected and functioning. Normally, all rotation is controlled by the joystick, with the dialbox controlling translation, hither plane positioning and the magnification factor of the display. All motion and scale changes are continuous in this case.

Display Reset

^ Reset both molecules to their initial configurations.

m Reset the current molecule to its initial configuration.

Display Scaling

+ Increase the magnification factor of the display.

- Decrease the magnification factor of the display.

These commands are superfluous with the dialbox in operation.

Depth Clipping

h Accept a new hither plane position from the user.

y Accept a new yon plane position from the user.

z Enable/disable z-clipping.

x Enable/disable smooth z-clipping.

p Set the clipping planes at the extremes of the molecule.

Structure Manipulation

A Select molecule A for future operations.

B Select molecule B for future operations.

e Select both molecules for future operations.

v Render the current molecule in color.

w Render the current molecule in white.

o Remove the current molecule from the display.

g Display the status of the current molecule.

Miscellaneous

n Accept a new site point from the user.

i Select the resolution of the display. The high resolution display is stationary, and should be used when still photographs are taken.

t Toggle between rotation about the center of the display, and the center of the current molecule.

= Display the current viewing parameters.

? Display the command list accepted by SPHERE.

q Exit SPHERE.

Displaying two structures

Owing to limitations in the user interface of SPHERE, the following procedure must be followed to display two molecules **using a common scale**:

1. Using CONMERGE or STICK, combine the two structure files into a common file. This serves to translate the individual structures into a common coordinate system.

2. Using KEEP, indicate that the intermediate files should be retained. This ensures that the SPHERE input file(s) will not be deleted.

3. Invoke SPHERE, specifying the atom sphere representation desired.

4. Exit SPHERE, then exit MMADS.

5. Edit the SPHERE input file (file suffix _.SPH) to insert a second molecule descriptor line. This is a line with an "m" in the first column, and a title starting in column _#3. This should be placed after the last atom entry for the first structure.

6. (Re)enter MMADS, then (re)enter SPHERE. The existing (edited) input file will be used for the display.

As designed, SPHERE permits the user to split a molecule into (up to) nine groups, allowing individual groups to be selected as well. This feature does not seem to work at this time. The maximum number of atoms that can be displayed is 700, and the user will be informed when merged structures exceed this limit. The user is directed to the Sphere-3000 documentation provided by Intermetrics if additional information is required.

3.6.6 C3D (CBM VAX-11/730 Only)

C3D allows the user to display an arbitrary electrostatic isopotential surface generated from the data calculated by the ELESTA command. This code was developed by George Purvis and Chris Culberson at the Quantum Theory Project at the University of Florida, Currently, the C3D only supports the Adage 3000 raster graphics engine as a display device. C3D prompts the user for several pieces of information:

Is FSS already in place (Y/N) [Y]:

which allows the user to indicate whether the Adage Fortran Support System has already been downloaded to the Adage,

Enter view orientation [0,0,0]:

which expects the x-, y- and z- rotation angles used to determine the display orientation. If all rotation angles are zero, the orientation of the current structure file is used. Due to limitations within C3D, rotation angles must be in the range [-90,90]. Finally, the user is prompted:

Enter contour level [0.05]:

which expects the absolute magnitude of the isopotential surface. As the data generated by the ELESTA command is in the form of a 3-D grid of points, C3D can be used repeatedly to display various isosurfaces. The electrostatic isopotential surface is color-coded by gradient, and the surface area of the positive and negative isosurface is displayed for the user.

3.6.7 MODRAW

MODRAW is DRAW Version 1.92 (as provided in the MOPAC distribution), integrated into MMADS. It only supports Tektronix 4010 and 4105 terminals as a graphics device, and requires an archive file (file suffix _.ARC) produced by MOPAC for operation. Several different plotting capabilities are available, and the user is referred to the DRAW documentation for additional information.

3.7 Theoretical Calculations

These commands allow the user to perform theoretical calculations using several semi-empirical methodologies. Owing to the computational intensity of these programs, the user should ALWAYS submit any calculations as batch jobs. While this may result in delays, the other users of the VAX will be most appreciative.

At this time, two theoretical programs are integrated into MMADS: INDO/S, developed by Zerner et al at the Quantum Theory Project at the University of Florida and MOPAC, developed by J. Stewart at the U. S. Air Force Academy. Through the use of commands such as ZCON and INTERNAL, MMADS allows the user to generate data sets for submission to the ab initio programs Gaussian-80 (UCSF) and Gaussian-82, as well as recover structure files from the resulting output files.

3.7.1 ZINDO

ZINDO allows the user to perform semi-empirical calculations on the current structure file using the INDO/S methodology. As currently implimented, ZINDO can perform a SCF calculation using the current molecular geometry, or optimize that geometry at the HF level. The user can specify the charge and multiplicity for the calculation, along with the particular semi-empirical approximation to use. In order to calculate the electrostatic potential for a structure file, ZINDO must be used to create the molecular wavefunction and density matrix. The user is referred to the ZINDO documentation if additional information is desired.

ZINDO prompts the user for several pieces of information:

Enter the net charge for the molecule:

which expects the net charge to be used in the calculation, and

Enter the multiplicity of the molecule:

which expects the multiplicity to be used in the calculation. Both the charge and multiplicity must be specified using integer values, with the multiplicity being greater than zero. Next ZINDO prompts:

Stationary (0) or Optimization (1) [1]:

which allows the user to specify whether the structure is to be optimized. If an optimization has been selected, ZINDO prompts:

Optimization resolution (High/Low) [LOW]:

which allows the user to specify whether the convergence criterion for the optimization should be reduced by an order of magnitude,

Integral Approximation [4 - INDO/2]:

which allows the user to specify the semi-empirical method to use, and

Interactive, Batch, Fast or Defer [BATCH]:

which allows the user to specify whether the calculation is to be performed at the user's terminal, submitted to the system batch or fast batch queue or deferred. The user is encouraged to perform all ZINDO optimizations in the background, on account of the large amount of computational effort required.

3.7.2 MOPAC

MOPAC allows the user to perform semi-empirical calculations on the current structure file using the MOPAC (V3.1) methodology. As currently implimented, MOPAC expects an input file (file suffix _.MNI) in the appropriate format. This file can be created using the VAX/VMS Editor, or using the XYZ command. If found, the calculation is carried out, creating an output file (file suffix _.MNO) that contains a description of the input data and results. If a successful optimization was performed, an archive file (file suffix _.ARC) is created as well. The user is referred to the MOPAC documentation if additional information is desired.

MOPAC prompts the user:

Interactive, Batch, Fast or Defer [BATCH]:

which allows the user to specify whether the calculation is to be performed at the user's terminal, submitted to the system batch or fast batch queue or deferred. The user is encouraged to perform all MOPAC optimizations in the background, on account of the large amount of computational effort required.

3.8 VAX/VMS DCL Commands

MMADS allows the user to execute a subset of the VAX/VMS DCL command language, to (hopefully) eliminate the need to exit and reenter MMADS during the course of a terminal session. The subset chosen attempts to include the "useful" commands, while excluding those that either would adversely affect the operation of MMADS or should be denied to the typical user.

The currently supported commands are:

COPY	Copy one file to another.
DELETE	Delete files from disk.
DIFFERENCE	Compare two files for differences.
DIRECTORY	List the contents of a directory.
LOGOUT	Logoff the VAX.
PHONE	Talk to another user on the VAX.
PRINT	Send a file to the VAX printer.
PURGE	Remove old copies of files on disk.
RENAME	Rename one file to another.
SEARCH	Search a file for a character string.
SET	Set process parameters.
SHOW	Display system information.
TYPE	Copy a file to the terminal.

In addition, two VAX/VMS utility programs (CBM/CRDEC only) are available:

FREE	Display the number of free blocks on disk.
TALK	Send a line of text to another user.

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APPENDIX A: STRUCTURE FILE INTERNAL FORMAT

This file is the central data structure of MMADS, containing molecular information that is required to execute any MMADS command. To use the EDIT command properly, the user is expected to understand the format of the individual entries in the file (these have been provided as FORTRAN format fields). The data records contained in the structure file are:

Record #1-	the header record for the file.
Column Nos. 1-3 (i3)	The number of atoms contained in the file.
Column Nos. 4-72 (a)	The title of the structure file.
Record #2 on -	the descriptions of the individual atoms.
Column No. 1 (1x)	blank
Column Nos. 2-3 (a)	The atom symbol. Single letter labels must be preceded by a space.
Column Nos. 4-8 (i5)	The atom index.
Column Nos. 9-20 (f12.6)	The x-coordinate.
Column Nos. 21-32 (f12.6)	The y-coordinate.
Column Nos. 33-44 (f12.6)	The z-coordinate.
Column Nos. 45-49 (i5)	The atom type (see below).
Column Nos. 50-79 (6i5)	The bond connectivity.

MMADS uses the atom type to encode information describing the molecular environment of each atom. Various commands utilize this information to distinguish between identical atoms in different molecular environments, thus providing a better representation for the user. The atom types used by MMADS are:

Atom Type	Description
1	sp3 Carbon
2	sp2 Carbon
3	Carbonyl Carbon
4	sp Carbon
5	Hydrogen
6	sp3 Oxygen
7	sp2 Oxygen
8	sp3 Nitrogen
9	sp2 Nitrogen
10	sp Nitrogen
11	Fluorine
12	Chlorine
13	Bromine
14	Iodine
15-18	Sulfur (this is still under development)
19	Silicon
20	unused
21	Alcoholic Hydrogen (N-H, O-H)
22	Cyclopropane Hydrogen
23	Amine Hydrogen
24	Carboxyl Hydrogen
25	Phosphorus
26-27	unused
28	Vinyl Alcohol Hydrogen

APPENDIX B: COMMON MMADS FILE SUFFIXES

During the course of a MMADS session, many intermediate files can be created. In addition, several of the MMADS commands produce output files for the user. The use of distinctive filename suffixes provides a means of identifying the contents and purpose of individual files (and is an extension of the VAX/VMS naming convention). Typical filename suffixes are:

.A	MM2 work file
.A1	MM2 work file
.ALI	MM2 input file
.ARC	MOPAC archive file
.ATB	MM2 angle energy file
.BBD	BBD output file
.BIN	BS3 input file
.BOU	BS3 output file
.BS3	BS3 optimized output file
.BTB	MM2 bond energy file
.CCT	CONOLLY contact surface file
.CEL	ELESTA output file (CONOLLY)
.CON	MMADS structure file
.CPT	CONOLLY work file
.CRN	CONOLLY reentrant surface file
.CRV	ELESTA work file
.CRY	CRYSTAL input file
.DAT	CHEMLAB structure file (or VAX/VMS generic data file)
.DEN	MOPAC density matrix file
.DRC	MIOPAC dynamic reaction coordinate file
.ELS	ELESTA output file
.ELS_OUT	ELESTA log file
.END	MOPAC terminator file
.F01	CONOLLY/UNIQUE/OVERLAP work file
.F02	CONOLLY/UNIQUE/OVERLAP work file
.F03	CONOLLY/UNIQUE/OVERLAP work file
.F07	CRUDE work file
.FCH	MMADS formal charge file

.GPT	MOPAC work file
.HYD	HYDRATE output file
.IMP	ELESTA work file
.INT	BS3/INTERNAL work file
.ITR	ZINDO optimization iteration record file
.JOB	Batch job file for submission
.LOG	Batch job log file
.MM2	MM2 answer file
.MNI	MOPAC input file
.MNO	MOPAC output file
.MRK	MMADS terminal type definition file
.NAM	CONMMI work file (archaic)
.NEW	MMADS work file
.PLS	CONOLLY work file
.PNT	ELESTA work file
.PLU	PLUTO input file
.PNT	CONOLLY work file
.PRM	MM2 geometric parameter file
.RES	MOPAC restart file
.RK2	ZINDO work file
.RKK	MMADS work file
.RWT	SURROUND work file
.SCP	MMADS script file
.SKE	SKETCH work file
.SMI	SMILES work file
.SPH	SPHERE input file
.SUB	MMADS command file
.TEM	ELESTA work file
.TMP	Temporary file (MMADS and VAX/VMS)
.TTB	MM2 torsional energy file
.Txx	ZINDO work file (where xx is an integer)
.ZHS	ZINDO work file
.ZNB	ZINDO basis set file
.ZND	ZINDO input file
.ZNE	ZINDO eigenvalue file
.ZNO	ZINDO output file

.XYZ	XYZ output file

Some of the intermediate files that are produced by MMADS do not follow the convention described above. These files are specific to internal MMADS operations, and many only appear in the user's directory after MMADS errors. A collection of these filenames is given below:

cdraw.wrk	KWIKDRAW intermediate file
contact.dat	CONOLLY working file
defer.com	MMADS file accumulating deferred batch jobs
filelist.txt	SPHERE input file
files.tmp	FILES working file
reentrant.dat	CONOLLY working file
sketch.	SKETCH screen image file
sorted.dat	CONOLLY working file
struc.dat	MMADS structure file record file
ztran.ztr	ZTRANSLATE output file

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AREA	Calculates the surface area of the current molecule (in A_^2), and determines the percentage of the surface of each atom that is exposed. AREA provides the user with the option of specifying the radius of the solvent molecule - which provides a means of calculating the surface area of a solvent/solute aggregate.
BBD	Calculates the "nearest neighbor" bond lengths, angles and torsionals of the current structure file. "Nearest neighbors" are defined as two atoms separated by (at most) the user-specified fraction of their respective covalent radii.
BELL	Rings the terminal bell. This is useful when generating script files for attracting the attention of the user.
BS3	Optimizes the current structure file, using the MM2 parameters with the Bigstrain-3 program obtained from Merck/QCPE.
BUDEDIT	Provides a means for editing the parameter file(s) required by MM2. Using BUDEDIT, the user can add, edit or delete specific bond stretch, bend or torsional modes.
C3D	Displays the electrostatic isopotential surface of the current structure file on the Adage 3000 raster graphics device. C3D assumes that ELESTA has been used to create the necessary data files. This command is specific to the CBM VAX-11/730.
CENCON	Centers the current structure file at the origin.
COMMANDS	Lists the current commands on the user's terminal.
COMMENT	Sends the user's comment(s) as mail to the MMADS custodian and/or developer.
CONBREAK	Separates a meta-structure file (containing more than one distinct structure) into individual structure files.
CONE	Calculates the Tolman Cone Angle for the specified atom triplet.
CONMERGE	Allows the user to create a meta-structure file, providing the means to align the individual structures using a common coordinate system.
CONOLLY	Calculates and displays Solvent Accessable surfaces on the user's terminal. These surfaces can be color-coded by atom type, formal charge or electrostatic potential.

COPY	The DCL copy command.
CPK	Minimizes the current structure file using a simple force field comprised of bond-stretch and non-bonded interactions.
CUDE	Performs an MM2 minimization on the current structure file, redefining all heavy atoms as carbons and all other atoms as hydrogens.
CRYSTAL	Allows the user to create structure files from crystal coordinates.
CVTCON	Converts structure files between MMADS and CHEMLAB (V5.0) format.
DELETE	The DCL delete command.
DELHYDROGENS	Removes all hydrogens from the current structure file.
DEVICE	Allows the user to specify the current graphics device type (currently, the user's terminal).
DIFFERENCE	The DCL difference command.
DIRECTORY	The DCL directory command.
DISABLE	Allows the user to turn off various MMADS options.
DRAW	Generates a rough drawing of the current structure file, using the atom indices or labels.
EDIT	The MMADS structure file editor. EDIT allows the user to review or alter the current structure file, add or delete atoms, generate standard coordinates or change the title line.
EIGEN	Experimental command that generates various structural descriptors for the current structure file.
ELECTOP	Uses the current structure file's geometry and formal charges to calculate Kaliszan's electronic descriptor (*Chromatog.* **2**,19(1987)).
ELESTA	Calculates the Electrostatic Isopotential Surface for the current structure file. Before ELESTA can be run, a stationary ZINDO calculation must be done to generate the necessary electronic information. The Adage 3000 is the only graphics device that is currently supported (via C3D).
EMPIRICAL	Provides the molecular and empirical formulae for the current structure file.
ENABLE	Allows the user to turn on various MMADS options.

EXECUTE	Runs the script files, using the specified structure filenames.
EXIT	Exit MMADS.
FILES	Lists the structure files (and versions) in the current (sub)directory.
FREE	Lists the amount of free disk space on the system.
GENHYDROGENS	Adds hydrogen atoms to the current structure file to fill "standard" valence on each atoms. It is assumed that the atom types are correct.
GPXSKETCH	Provides a means of graphical structure input, using the mouse and display of the DEC uVAX-II/GPX.
GVOLUME	Calculates the molecular volume using a grid approximation. This is a preliminary version of what will eventually be an elaborate command that maps pharmacophores.
HELP	Provides on-line help for MMADS.
HYDRATE	Provides distance and neighbor information on the water molecule(s) surrounding a non-water molecule, using the current structure file (which must be a meta file).
INCREMENT	Adds the user-specified increment to the current structure filename (1 if omitted).
INTERNAL	Generates a rough internal coordinate file, for use with MOPAC (AMPAC), Gaussian82 and Gaussian80 (UCSF).
KEYPAD	Enables command selection by keypad key.
KWIKDRAW	Allows the user to create structure files from molecular connectivity. This is the standard structure input routine for MMADS.
LOGOUT	Cleans up many of the work files created by MMADS, and logs the user off the system.
MIRROR	Produces a mirror-image of the current structure file across the plane containing the user-specified axis.
MM2	Performs an MM2 minimization on the current structure file.
MODEL	The simplest minimization algorithm in MMADS. It provides a quick means of generating reasonable structures, and can handle structures of up to 999 atoms (the current limit of MMADS).

MODRAW	This is the MOPAC DRAW program, modified to run within MMADS. The user is referred to the MOPAC documentation for further information.
MOPAC	This is MOPAC V3.1, set up to run within MMADS.
MOPCON	Recovers a structure file from MOPAC (AMPAC) output files (the .mno and .arc files).
MSA	Calculates the volume shared between two oriented structures. This command is specific to CBM/CRDEC.
MVOLUME	Calculates the molecular volume, using an approximate numerical integration of each unique atomic region.
NEAREST	Alters the molecular connecivity to reflect "nearest neighbor" bonding (as defined in BBD above).
NEWMAN	Allows the user to generate Newman Projections of the current structure file.
NEWS	Allows the user to peruse the news file - a reverse chronology of the changes that have been made to MMADS.
PARAM	Queries the user for the MM2 parameter file to use.
PHONE	The DCL phone command.
PLUTO	A modified version of the Cambridge Crystallographic Database display program. PLUTO provides stick, ball-and-stick and solid representations of the current structure file.
PRINAX	Aligns the current structure file along its principle axes.
PRINT	The DCL print command.
PROCESS	Allows the user to specify the numeric suffix of the current structure filename (e.g. PROCESS 12, while using STRUCT2 would change the current structure filename to STRUCT12).
PURGE	The DCL purge command.
RENAME	The DCL rename command.
RESET	Resets the Adage 3000 raster graphics engine. This command is specific to the CBM VAX-11/730.
SCRIPT	Allows the user to create a script file (a file of MMADS commands to be run in sequence).
SEARCH	The DCL search command.

SET	The DCL set command.
SHARED	Calculates the volume shared between two oriented molecules, using the approximate numerical integration technique of MVOLUME.
SHOW	The DCL show command.
SKETCH	Is an early version of the SKETCH command of QUIPU (developed by George Purvis at the Quantum Theory Project at the University of Florida). SKETCH allows the user to enter structures using the ANSI terminal's graphics capabilities.
SMILES	Allows the user to enter a structure using SMILES notation (as with CLOGP).
SPHERE	Allows the user to display the current structure file on the Adage 3000 raster graphics engine using SPHERE 3000. This command is specific to the CBM VAX-11/730.
STATUS	Provides the user with information on the current status of various flags within MMADS.
STICK	Enables the user to generate stick, ball-and-stick and solid representations of up to ten structures. Atoms can be labeled by label or formal charge. The MM2 answer file can be used to label the bond, angle or torsional strain in the current structure file. The display can be saved as a (meta) structure file for later processing.
STRETCH	Allows the user to alter the geometry of the current structure file by a user-specified multiplication factor along each cartesian axis (individually).
SURROUND	Allows the user to surround the current structure file with an arbitrary number of water molecules in an arbitrary orientation.
TALK	Allows the user to send a message to another terminal.
TMODELER	An earlier version of the MODEL program developed by Clark Still.
TRIQUI	Converts structure files between MMADS and QUIPU format.
TYPE	The DCL type command.
USE	Allows the user to specify the structure filename to use.
VECTOR	Experimental command that generates various electronic descriptors for the current structure file. VECTOR requires a Formal Charge charge file for operation.

VOLUME	Calculates the volume of the current structure file (in A^3). This command is specific to CBM/CRDEC.
WATER_SHELL	Generates a shell of 14 water molecules at the vertices and and the centers of each face of a rectangular prism surrounding the current structure file. This is also from QUIPU.
WEIGHT	Calculates the molecular weight of the current structure file.
WHERE	Lists the name of the current (sub)directory.
XYZ	Generates a cartesian coordinate file from the current structure file, suitable for use with MOPAC (AMPAC) via the XYZ input option.
ZCON	Generates a structure file from a Z-matrix extracted from the output file from Gaussian80 (UCSF) or Gaussian82.
ZINDO	Submits the current structure file to the INDO/S program developed by Michael Zerner (et al) at QTP. This is an excellent semi-empirical program (CNDO and INDO), but it must be obtained directly from Dr. Zerner.
ZTRANSLATE	Extracts z-matrices from a G80 (UCSF) output file, and creates data files suitable for (re)submission to G80 (UCSF).

APPENDIX D: MMADS GENERIC GRAPHICS LIBRARY

The MMADS Generic Graphics Library resulted from the need to create a small, easily modified, device-independent graphics library. Such a library would enable the developers of MMADS to maintain a single version of code for each of the graphics commands in MMADS, as all machine-dependent code would be contained in the graphics library (transparent to the programmer).

At this point, three graphics devices are supported: the Tektronix 4010 and 4105 terminals, along with hardware that emulates either of these devices, and the Digital Equipment Corporation uVAX-II/GPX 2-D color workstation. Future development will include support for the Adage 3000 raster graphics system and the Silicon Graphics IRIS color workstations. Obviously, the 3-D color workstations provide greatly enhanced hardware capabilities as compared to the Tektronix terminals (and the GPX), but all future versions of the MMADS Generic Graphics Library will remain compatable with this implementation.

Available Commands

clear_dialog — Clear Dialog (Text) Screen

call: call clear_dialog

calling parameters: none

This subroutine clears the dialog (text) area of the display.

clear_grafix — Clear Graphics Screen

call: call clear_grafix

calling parameters: none

This subroutine clears the graphics area of the display.

draw_circle — Draw a Circle

call: call draw_circle(x,v,radius,number,fill,border)

calling parameters:

x origin x-coordinate (internal coordinates)
y origin y-coordinate (internal coordinates)
radius circle radius (internal coordinates)
number number of line segments to use to draw circle
fill fill pattern to use (if available)
border = yes_value, include the border
# yes_value, exclude the border

This subroutine draws a circle centered at (x,y), with a radius of <radius>, using <number> line segments. The value of <fill> specifies whether the circle will be empty, or filled with the specified fill pattern. The value of <border> specifies whether the circle will be drawn with a border.

draw_poly Draw a Polygon

call: call draw_poly(x,y,number,fill,border)

calling parameters:

x origin x-coordinate (internal coordinates)
y origin y-coordinate (internal coordinates)
number number of points defining the polygon
fill fill pattern to use (if available)
border = yes_value, include the border # yes_value, exclude the border

This subroutine draws a polygon with <number> vertices, starting at (x(1),y(1)) and ending at (x(number),y(number)). The value of <fill> specifies whether the polygon will be empty, or filled with the specified fill pattern. The value of <border> specifies whether the polygon will be drawn with a border.

draw_to Draw a Line

call: call draw_to(x,y)

calling parameters:

x point x-coordinate (internal coordinates)
y point y-coordinate (internal coordinates)

This subroutine draws a line from the current cursor position to (x,y).

enter_grafix — Enable Graphics Device

call: call enter_grafix(lun,device)

calling parameters:

lun graphics device logical unit number
device = t4105, graphics device is a Tek 4105
= t4010, graphics device is a Tek 4010
= GPX, graphics device is a uVAX-II/GPX

This subroutine initializes the MMADS Generic Graphics Library. It is assumed that the calling routine has ensured that the graphics device is linked to <lun>, which will be used for all graphics i/o. <device> specifies the graphics device type.

exit_grafix — Disable Graphics Device

call: call exit_grafix

calling parameters: none

This subroutine disables the MMADS Generic Graphics Library, and resets the graphics device to ANSI mode.

flush — Flush Graphics I/O Buffer

call: call flush

calling parameters: none

This subroutine flushes the i/o buffer used by the MMADS Generic Graphics Library. This should be done after the calling program has completed a plot, to ensure that all of the information is sent to the display.

frame — Frame Graphics Display

call: call frame(xmin,xmax,ymin,ymax,type)

calling parameters:

xmin	minimum internal x-coordinate
xmax	maximum internal x-coordinate
ymin	minimum internal y-coordinate
ymax	maximum internal y-coordinate
type	type of framing to use

This subroutine sets the x and y coordinate ranges that will be used to map internal coordinates to the hardware pixel addresses, along with the type of framing (square or rectangular) to use.

line_color — Set Graphics Line Color

call: call line_color(color)

calling parameters:

color desired line color (integer in the range [0,7])

This subroutine sets the line color to be used by draw_to, draw_circle and draw_poly. The programmer is referred to the

appropriate hardware manual for a description of the available color codes.

line_style — Set Graphics Line Style

call: call line_style(style)

calling parameters:

style desired line style

This subroutine sets the line style to be used by draw_to. Currently, this routine supports only two styles: solid (style = 0) and dotted (style = 4) lines.

move_to — Move the Cursor

call: call move_to(x,y)

calling parameters:

x point x-coordinate (internal coordinates)
y point y-coordinate (internal coordinates)

This subroutine sets the current cursor position to (x,y).

output_text — Write Text on the Graphics Screen

call: call output_text(x,y,string,length)

calling parameters:

x x-coordinate of text (internal coords)
y y-coordinate of text (internal coords)
string text to be written
length number of characters in <string>

This subroutine writes the specified text string on the graphics screen at (x,y).

rgb__color Set an Entry in the Color Map (RGB)

call: call rgb__color(index,red,green,blue)

calling parameters:

index the color index to set
red the red fraction
green the green fraction
blue the blue fraction

This subroutine sets the RGB indices for the specified color index (fractions in the range [0.0,1.0]. This enables the programmer to alter the default color settings of the graphics device, based on the specific requirements of the graphics application. It is strongly suggested that the programmer restore all color indices to their default setting before exiting.

scale__x Map Internal X-Coordinate to a Pixel Address

call: call scale__x(x)

calling parameters:

x internal x-coordinate

This integer function returns the hardware pixel address corresponding to <x>, using the internal coordinate system defined via the FRAME command. Values of <x> outside the range [xmin,xmax] will be set to the appropriate extremum value. SCALE__X assumes that the display area is a square, and performs the mapping function accordingly (using the pixel address range of the graphics device).

scale__y — Map Internal Y-Coordinate to a Pixel Address

call: call scale__y(y)

calling parameters:

y internal y-coordinate

This integer function returns the hardware pixel address corresponding to <y>, using the internal coordinate system defined via the FRAME command. Values of <y> outside the range [ymin,ymax] will be set to the appropriate extremum value. SCALE__Y assumes that the display area is a square, and performs the mapping function accordingly (using the pixel address range of the graphics device).

surface__color — Set an Entry in the Color Map (HLS)

call: call surface__color(index,hue,light,satur)

calling parameters:

index the color index to set
hue the hue index (HLS coding)
light the lightness index (HLS coding)
satur the saturation index (HLS coding)

This subroutine sets the HLS indices for the specified color index. This enables the programmer to alter the default color settings of the graphics device, based on the specific requirements of the graphics application. It is strongly suggested that the programmer restore all color indices to their default setting before exiting.

text__color — Set Graphicstext Color

call: call text__color(color)

calling parameters:

color desired text color (integer in the range [0,7])

This subroutine sets the color that will be used for text written by output_text. As with surface_color, it is strongly suggested that the programmer restore the text color to white befor exiting.

write_mode Set Graphicstext Writing Mode

call: call write_mode(mode)

calling parameters:

mode = 1, replace existing display
= 0, overstrike existing display

This subroutine specifies whether text written by output_text replaces or overstrikes the existing display. As with surface_color, it is strongly suggested that the programmer set the graphics terminal to overstrike mode before exiting.

APPENDIX E: MMADS GRAPHICS PRIMITIVE LIBRARY

The MMADS Graphics Primitive Library contains the subroutines that perform the actual hardware operations on the graphics device. As such, these routines can be called from the graphics application directly, but it is strongly suggested that the MMADS Generic Graphics Library be used as an interface. Two graphics devices are supported: the Tektronix 4010 and 4105 terminals.

The Primitive Library was designed with an eye towards simplicity - Each subroutine contains the code necessary to perform only a single graphics operation. The subroutine name can be broken down into two parts: the device type, TEK (Tek 4105) or P10 (Tek 4010), and the mnemonic for the operation, such as SLI (for Set Line Index). As additional graphics devices are added, this naming convention will be expanded to segregate the primitives.

In order to improve the performance of the graphics application, all i/o requests are buffered and sent to the graphics device using large, unformatted write operations. This greatly reduces both the operating system and Fortran Format processing overhead. This feature is only implemented for the Tektronix 4105 terminal.

Available Primitives (Tek 4105)

tekbpb — Begin Panel Boundary

call: call tekbpb(ix,iy,incl)

calling parameters:

ix	pixel x-coordinate
iy	pixel y-coordinate
incl	= 1, include the panel boundary
	= 0, exclude the panel boundary

This routine marks the start of a panel on the graphics screen, and specifies whether the panel will be drawn with a boundary.

tekcrd — Generate a Coordinate String

call: call tekcrd(ix,iy,array)

calling parameters:

ix pixel x-coordinate
iy pixel y-coordinate
array bit string to send to the terminal

This subroutine constructs the five byte bit string required to specify a pixel address on the graphics screen.

tekdcl — Clear Dialog Screen

call: call tekdcl

calling parameters: none

This subroutine clears the dialog area of the display.

tekdrw — Draw a Line

call: call tekdrw(ix,iy)

calling parameters:

ix pixel x-coordinate
iy pixel y-coordinate

This subroutine draws a line from the current cursor position to (ix,iy).

tekepn — End a Panel Definition

call: call tekepn

calling parameters: none

This subroutine indicates that the current cursor position is the last

point in a panel, forcing a line connecting this point with the point specified by TEKBPB. Any panel defined using TEKBPB/TEKEPN will be a closed polygon, filled with the current fill pattern.

tekfls — Flush Graphics Buffer

call: call tekfls

calling parameters: none

This subroutine flushes the graphics buffer, and should be called at the end of each plot to ensure that all information has been sent to the graphics screen.

tekgcl — Clear Graphics Screen

call: call tekgcl

calling parameters: none

This subroutine clears the graphics area of the display.

tekint — Generate an Integer String

call: call tekint(integ,tint,ntint)

calling parameters:

integ integer to be encoded
tint bit string to send to the terminal (in reverse order)
ntint number of characters in <tint>

This subroutine constructs the variable-length bit string required to encode an integer to send to the graphics terminal.

tekmod Set Graphics Terminal Mode

call: call tekmod(mode)

calling parameters:

mode = 0, set TEK mode (graphics)
= 1, set ANSI mode (VT100)

This subroutine sets the operating mode for the graphics terminal to TEK (graphics) or ANSI (VT100) mode. The programmer is referred to the appropriate hardware manual for a description of the commands available in each mode.

tekmov Move the Cursor

call: call tekmov(ix,iy)

calling parameters:

ix pixel x-coordinate
iy pixel y-coordniate

This subroutine sets the current cursor position to (ix,iy).

tekout Perform Buffered I/O to the Graphics Device

call: call tekout(length,string)

calling parameters:

length the number of bytes in <string>
string the escape sequence to send to the terminal

This subroutine concatenates all Tek 4105 escape sequences, sending output to the graphics LUN (assumed to be open) in large, unformatted blocks. This greatly reduces the i/o overhead incurred

by the graphics application.

tekrst — Reset the Color Setting

call: call tekrst

calling parameters: none

This subroutine resets the hardware color wheel to the factory default settings, and sets the line color for the graphics screen to white. The programmer is referred to the appropriate hardware manual for a description of the default colors.

tekscm — Set Surface Color Map Entry

call: call tekscm(index,hue,light,satur)

calling parameters:

index	color index to be redefined	
hue	HLS hue index	(integer)
light	HLS lightness index	(integer)
satur	HLS saturation index	(integer)

This subroutine resets the HLS indices associated with the specified color index.

teksfp — Select Fill Pattern

call: call teksfp(icolor)

calling parameters:

icolor color index or hardware dither pattern index

This subroutine sets the fill pattern (solid color or dither pattern)

to be used when drawing panels. The programmer is referred to the appropriate manual for a description of the available dither patterns.

teksgawm — Set Graphics Area Writing Mode

call: call teksgawm(mode)

calling parameters:

mode = 0, replace existing display
= 1, overstrike existing display

This subroutine specifies whether text written on the graphics screen replaces or overstrikes the existing display.

teksli — Set Line Index

call: call teksli(color)

calling parameters:

color color index to use (integer)

This subroutine sets the line color to be used on the graphics screen.

teksls — Set Line Style

call: call teksls(code)

calling parameters:

code = 0, use solid lines (_____) = 4, use dotted lines (. . .)

This subroutine sets the line style to be used on the graphics

screen. The programmer is referred to the appropriate manual for a description of the available line styles.

teksti — Set Text Index

call: call teksti(color)

calling parameters:

color color index to use (integer)

This subroutine sets the color for text written on the graphics screen.

tekwrt — Write Text on the Graphics Screen

call: call tekwrt(ix,iy,string,length)

calling parameters:

ix pixel x-coordinate
iy pixel y-coordniate
string text to be written
length number of characters in <string>

This subroutine writes the specified text string on the graphics screen at (ix,iy).

Available Primitives (Tek 4010)

p10crd — Generate a Coordinate String

call: call p10crd(ix,iy,array)

calling parameters:

ix pixel x-coordinate
iy pixel y-coordinate
array bit string to send to the terminal

This subroutine constructs the four byte bit string required to specify a pixel address on the graphics screen.

p10dcl — Clear Dialog Screen

call: call p10dcl

calling parameters: none

This subroutine clears the dialog area of the display.

p10drw — Draw a Line

call: call p10drw(ix,iy)

calling parameters:

ix pixel x-coordinate
iy pixel y-coordinate

This subroutine draws a line from the current cursor position to (ix,iy).

p10gcl — Clear Graphics Screen

call: call p10gcl

calling parameters: none

This subroutine clears the graphics area of the display.

p10mod — Set Graphics Terminal Mode

call: call p10mod(mode)

calling parameters:

mode = 0, set TEK mode (graphics)
= 1, set ANSI mode (VT100)

This subroutine sets the operating mode for the graphics terminal to TEK (graphics) or ANSI (VT100) mode. The programmer is referred to the appropriate hardware manual for a description of the commands available in each mode.

p10mov — Move the Cursor

call: call p10mov(ix,iy)

calling parameters:

ix pixel x-coordinate
iy pixel y-coordniate

This subroutine sets the current cursor position to (ix,iy).

p10sls — Set Line Style

call: call p10sls(code)

calling parameters:

code = 0, use solid lines (_____)
= 4, use dotted lines (. . .)

This subroutine sets the line style to be used on the graphics screen. Due to compatability restrictions, the style codes indicated above are translated to the actual hardware values. The

programmer is referred to the appropriate manual for a description of the available line styles.

p10wrt — Write Text on the Graphics Screen

call: call p10wrt(ix,iy,string,length)

calling parameters:

ix pixel x-coordinate
iy pixel y-coordniate
string text to be written
length number of characters in <string>

This subroutine writes the specified text string on the graphics screen at (ix,iy).

APPENDIX F: MMADS INPUT PARSER

The MMADS Input Parser can be broken down into three parts: a routine to get a token from an input string (either space or comma terminated), a routine to compare a token against a list of commands and a routine to decode a token to a real number or a collection of integers.

These three routines are used by STICK (and throughout the MMADS code that has been written at CRDEC) to provide a consistent and straightforward user-interface. Commands can be entered in either upper or lower case, and abreviations are acceptable. The user is informed if an abbreviated command is ambiguous.

Parsing Routines

parse — Get a Token from a String

call: ierr=parse(string,length,token,len2)

calling parameters:

string input string, returned with token removed
length length of <string>, returned with token removed
token token removed from <string>
len2 length of <token>
ierr termination code: = 0, normal return
= 1, EOL terminated

= 2, null token (len2 = 0)

This function accepts a string of length <length> from the caller, and scans for the first occurence of a space or a comma. If either are found, the characters preceeding the separator are returned as <token> with a length of <len2>, and removed from <string> (with <length> adjusted accordingly). The return code indicates whether <token> was found, and whether a separator or EOL was encountered.

parsec — Check Token against Command List

call: ierr=parsec(string,length,table,entry)

calling parameters:

string the token to be checked
length length of <string>
table command table, terminated by '*END*'
entry explicit command, returned to caller
ierr termination code: = 0, normal termination

= 1, invalid command

= 2, ambiguous command

This function accepts a string of length <length> from the caller, and compares it against the first <length> bytes of the character strings contained in <table>. The number of matches determine whether the command is valid, ambiguous or invalid. If <string> is a valid command, PARSEC returns the fully-specified command in <entry>.

parsen — Decode Token to Real/Integers

call: ierr=parsen(type,string,length,array,numb1, iarray,numb2,maxnum)

calling parameters:

type = 0, real number
= 1, integer number(s)
string character string to process
length length of <string>
array array containing real numbers
numb1 number of real numbers in <array> (currently, 1)
iarray array containing integers

numb2 number of integers in <iarray>
maxnum for integers, largest possible number
err termination code: = 0, normal return

= 2, invalid number string

This function accepts a character string of length <length>, and processes it according to the value of <type> passed by the caller. If integers are desired, "-" is treated as a dash (as in 5-10, 5 through 10), negative numbers are not permitted, and the maximum valid integer is <maxnum>. If a real number is desired, "-" is a minus sign, and a decimal point (if omitted) will be assumed to follow the last digit in <string>.

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APPENDIX G: INSTALLING MMADS

MMADS is distributed in two media formats: 9-track magnetic tape, written at 1600 bpi and TK50 cartridge tape. Both contain two backup save sets, one containing the source and build files and the other containing the executable and command files. If no changes are planned for MMADS, the source save set need not be read from tape.

To install the executable and command files for MMADS, the following steps should be performed:

1. Create a master directory [MMADS] on a user volume. All of the files needed to use MMADS will reside in subdirectories of this master directory.

2. Set the current (default) directory to [MMADS], and mount the MMADS distribution tape as a foreign volume.

3. Using BACKUP, restore all of the files in the executable and command files save set:

   $ BACKUP <tape>:MMADS.BCK *

   where <tape> is the appropriate device name for the magnetic tape drive.

4. Once all files have been copied to disk, set the file ownership and/or protection as appropriate.

5. Include the following DCL commands into the login file for each potential MMADS user (or the system-wide login file):

```
$ MM*ADS  :==      @<disk>:[MMADS.COM]MMADS
$ DEFINE TRB$COMMAND  <disk>:[MMADS.COM]
$ DEFINE TRB$SYSTEM   <disk>:[MMADS.EXE]
$ DEFINE TRB$HELP     <disk>:[MMADS.HLP]
$ DEFINE TRB$LIBRARY  <disk>:[MMADS.LIB]
$ TRB$DEFN  == "NO"
$ TRB$CLEAN  == "ON"
```

   where <disk> is the device name for the disk volume containing [MMADS]. These commands define the DCL string required to enter MMADS, along with the four subdirectories required by MMADS.

6. Change the MMADS symbol definition file ([MMADS.COM]TRBDEF.COM) entries for TRB$CARETAKER to reflect the mailing address of the MMADS custodian and

TRB$PRINTER to reflect the device name for the system printer.

7. As a large number of files can be created during the course of a user's session, MMADS purges and/or deletes many of the work files created during the user's terminal session upon logout. If no cleanup is desired, change the value of TRB$CLEAN listed above to "OFF".

To install the source and build files for MMADS, the following steps should be performed:

1. Create a master directory [TRIBBLE] on a user volume. All of the files needed to recompile portions of MMADS will reside in subdirectories of this master directory.

2. Set the current (default) directory to [TRIBBLE], and mount the MMADS distribution tape as a foreign volume.

3. Using BACKUP, restore all of the files in the source and build files save set:

```
$ BACKUP <tape>:TRIBBLE.BCK *
```

   where <tape> is the appropriate device name for the magnetic tape drive.

4. Once all files have been copied to disk, set the file ownership and/or protection as appropriate. It is highly recommended that write access to the source and build files be restricted to those responsible for maintaining MMADS, in order to avoid unintentional alterations.

As MMADS is a system that is evolving as new mission needs are identified, some "bugs" in its operation are to be expected. Care has been taken to eliminate all errors, but feel free to contact us if/when any errors occur. Of course, if any corrections are made locally, please send them back so we can install them in our version.

We do ask that you refrain from further distributing the source code and executables of MMADS, referring such requests back to us. Even though MMADS is freely distributed, the authors are attempting to maintain source code integrity via this "gentleman's agreement". Given a list of sites, information concerning corrections and enhancements can be quickly distributed. If any enhancements or modifications to MMADS that you have made can be sent back to us, we can include these changes into the next release version.

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APPENDIX B: CUSTOMIZING MMADS

MMADS permits users to individually tailor its operation through the use of the customization option. This allows new commands to be tested and debugged before they are installed in MMADS, and permits users to alter the operation of existing commands to better meet their needs. This option eliminates the need for changing the files contained in MMADS and its subdirectories whenever program changes are being developed.

When CUSTOMIZATION is ENABLEd, MMADS looks for a customization file in the current (sub)directory with the filename MMADS.CUSTOM. This file contains all of the new/altered commands, along with the action to perform when each command is entered. The following format is used for each entry in MMADS.CUSTOM:

<command>#<DCL string>

where <command> is the new/altered MMADS command and <DCL string> is the command string required to execute the command. All command names contained in MMADS.CUSTOM must be specified in UPPER case.

Each time the user enters a command, MMADS first checks the contents of MMADS.CUSTOM to determine whether the command has been (re)defined. If the command is contained in the customization file, the DCL string associated with that command is used. The user is informed if the command is ambiguous or invalid, although it is important to note that ambiguity checking is not performed between the commands specified in MMADS.CUSTOM and the commands contained within MMADS.

If CUSTOMIZATION is ENABLEd, but MMADS is unable to find MMADS.CUSTOM in the current (sub)directory, the user is informed and CUSTOMIZATION is DISABLEd. The user is informed upon entry whether MMADS has been customized.

Finally, a short summary of the directory structure for MMADS will be provided:

[MMADS] Master directory for the executable and command files.

[MMADS.COM] Subdirectory containing the command files.

[MMADS.EXE] Subdirectory containing the executables.

[MMADS.LIB] Subdirectory containing various library files.

[MMADS.HLP] Subdirectory containing MMADS manual and help files.

[TRIBBLE] Master directory for the source and build files.

[TRIBBLE.SOURCE] Subdirectory containing the source and include files.

[TRIBBLE.BUILD] Subdirectory containing the build files.

[TRIBBLE.OBJ] Subdirectory containing all object files.

[TRIBBLE.EXE] Subdirectory containing all executables.

[TRIBBLE.LIB] Subdirectory containing object library files.

APPENDIX I: USEFUL REFERENCES

Publicly available programs from several sources have been used in the creation of MMADS. The following list represents the origins of most of the source code not written in-house.

1. The Quantum Chemistry Program Exchange (QCPE)
   Department of Chemistry
   Indiana University
   Bloomington, IN 47405

   This is an excellent source of programs for all areas of Chemical Research. CONOLLY, MM2, BS3 and Gaussian-80 (UCSF) were obtained from QCPE and integrated into MMADS.

2. The Quantum Theory Project (QTP)
   University of Florida
   362 Williamson Hall
   Gainesville, FL 32611

   QTP is one of the largest and most active research groups in Theoretical Chemistry, both in the areas of formal methodology and application development. Dr. Michael Zerner has led a group that has developed INDO/S (integrated as ZINDO), which is an extremely versatile semi-empirical technique. Dr. George Purvis has developed several graphical display programs that have advanced the state of the art in Molecular Modeling (ELESTA, C3D).

3. The Frank J. Seiler Research Laboratory
   U.S. Air Force Academy
   Colorado Springs, CO 80840

   Dr. James Stewart has developed MOPAC, which is the "industry-standard" semi-empirical technique for modeling organic chemistry. Maj. Donn Storch developed the display program DRAW, which provides a user with a means of representing the atomic and elcctronic structure of a molecule.

4. Intermetrics, Inc.
   733 Concord Avenue
   Cambridge, MA 02138

   Intermetrics developed the Sphere-3000 display program.

5. Department of Chemistry
Carnegie-Mellon University
4400 Fifth Avenue
Pittsburgh, PA 15213

The reasearch group led by Dr. John Pople developed the Gaussian-82 ab initio quantum program.

6. Medicinal Chemistry Project
Pomona College
Claremont, CA 91711

The Medicinal Chemistry Project developed the C LOG P package.

7. Department of Chemistry Columbia University New York, NY 10027

Dr. Clark Still developed the MODEL package (integrated as TMODELER).

8. Crystallographic Data Centre
University Chemical Laboratory
Lensfield Road
Cambridge, England CB2 1EW

This group maintains the Cambridge Crystallographic Database.