THE
UCSD
MOLECULAR MODELING SYSTEM

REFERENCE MANUAL

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Revision History

Version 1.0 February 12, 1986

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CHAPTER 1

Introduction

The UCSD Molecular Modeling System (MMS) is a collection of software tools that allow the user to view and interact with dynamic computer generated line drawing displays of molecular structures. This manual is the first in a series of two manuals that document MMS. The second is the MMS Users' Guide, a tutorial introduction to its use and capabilities.

This manual contains detailed descriptions of all of the commands and options available in the MMS. The documents for each program or command are built from a common format of named sections. Not all of these sections are necessarily included in each document:

NAME
: gives a brief summary of the purpose or function of the subject

SYNOPSIS
: details the syntax of the command. **BOLDFACE** or underlined characters should be entered literally. Brackets ([]) indicate optional parameters. Other text are symbolic names for required parameters.

DESCRIPTION
: tells you how to use this command and the effects of the optional parameters.

FILES
: lists filenames that are built in to the program.

SEE ALSO
: lists other subjects that are related to the current subject.

BUGS
: documents known problems and deficiencies.

AUTHOR
: indicates the person responsible for your joy or grief.

CHAPTER 2

MMS Graphics System Requirements

Required Hardware

(1) Silicon Graphics IRIS 2400 or 2400 TURBO workstation with a minimum of 16 bitplanes.

Required Software

(2) Silicon Graphics software release GL2-Wx.3 or higher.

Hardware Recommendations

The following hardware is not required, but will enhance the performance and operation of the software.

(1) Floating point hardware. This option speeds up the real-time calculations within MMS. It also substantially reduces the execution time of off-line programs such as molecular surface generators and contouring programs.

(2) An auxiliary ascii terminal. If you log in and run MMS from a terminal other than the console, then messages sent to the terminal screen will not be intermixed (and possibly erased!) with the graphics.

(3) The Turbo option. Graphics programs such as MMS run at least twice as fast on the 2400 Turbo as on the 2400. Program compilation speeds up by at least a factor of 4. The 2400 Turbo with floating point accelerator executes floating point code on the order of 7 times faster than the 2400 with floating point hardware.

(4) Additional CPU memory. While MMS initially runs within the physical memory provided by a base model IRIS (currently 2 megabytes), as more models are added or more features are enabled the memory demands may exceed the available memory. The virtual memory features of the operating system will allow the program to continue running, but performance may be degraded. I recommend having at least 4 megabytes in your IRIS.

CHAPTER 3

MMS Installation Instructions

1. Login and set the working directory to a location in the filesystem where you want the MMS built. A subdirectory called *mms* will be created there. There should be approximately 2.5 megabytes of disk space available.
2. Insert the MMS tape cartridge into the tape drive and enter the command:

   tar xvo

   When the command prompt reappears the entire contents of the tape have been transferred to the disk. Remove the tape cartridge and store it in a safe place.
3. Move into the MMS subdirectory with the command:

   cd mms

4. Remove old programs and object code by running the shell script *clean.mms* with the command:

   clean.mms

   This step guarantees that the next step will recompile and regenerate every component of the UCSD MMS.
5. Run the shell script *install.mms* with the command:

   install.mms

   This script attempts to create system directories where MMS programs and data will reside. If you do not have permission to create them the script will generate an error message and stop. You will be told to log in as *root* and run the script *makedirs.mms*. Continue from this point by rerunning the shell script *install.mms*.
6. You will be asked if your IRIS has floating point hardware. Respond with **y** or **n** as appropriate for your machine. The rest of the installation is automatic. Commands will appear on the terminal screen as they are executed. The installation takes approximately 30 minutes on the 2400, and about 6.5 minutes on the 2400 Turbo.
7. When the command prompt reappears the UCSD MMS is installed and ready to run. The MMS programs reside in a directory called */usr/local/bin/mms*. This directory should be added to each MMS user's search path.

CHAPTER 4

Database Generation

The programs documented in this chapter are used to prepare data for display by the Molecular Modeling System. In order to display a line drawing molecular model, the MMS needs three kinds of information:

(1) The coordinates of the atoms, which determine where the lines are drawn.

(2) The connectivity (bonds) between atoms, so the MMS will know which atoms to draw lines between.

(3) The names of the atoms, so that they may be selected using a nomenclature familiar to the user.

This information is placed in a file called a *molecular description*. This file contains only ascii characters, and thus may be created, modified, and read by humans using available text editors. The format of this file is documented in the *MMS Reference Manual* in the description of the program NEWMOL.

The purpose of NEWMOL is to convert a file which is easily read by humans into a binary file which can be quickly processed by an interactive graphics program. These binary files are hereafter referred to as *MMS databases*. NEWMOL is used to generate MMS databases for relatively small molecules, such as amino and nucleic acids, and cofactors such as NAD. Many of these molecules are provided with the MMS distribution. See the NEWMOL description in this manual for a complete list. NEWMOL requires that every atom in the molecule have a unique name. While this is not a problem for small molecules, it becomes awkward to define meaningful names for any structure with more than a few dozen atoms.

Fortunately, we can take advantage of the fact that large macromolecules are for the most part composed of chains of simpler subunits. NEWMOL is first used to create a collection of subunit templates. A second program called MOLASM (MOLecular ASseMbler) takes as input a file of atomic coordinates in the Brookhaven Protein Data Bank format. For each subunit, MOLASM merges the connectivity and nomenclature from the template with atom data from the coordinate file, linking together the subunit databases into a macromolecular database.

Molecular models are not limited to line segments connecting atom centers. Another example of a molecular model is a set of electron density contours such as those produced by the program CONTOUR.

NAME

newmol -- generate new MMS database templates

SYNOPSIS

newmol < input

DESCRIPTION

NEWMOL is used to generate new database templates for use by the MMS Molecular Assembly program **MOLASM.** It also creates displayable MMS databases if atomic coordinates are included.

The input is read from the standard input as a text file describing the nomenclature, connectivity, and optionally, the coordinates of the atoms in the new molecule.

The output is an MMS molecular database, which is placed in a file whose name is specified by the RESIDU input record (see below). Note that since all names in MMS databases are uppercase, the output filename will also be forced to uppercase before the file is created.

CREATING THE MOLECULAR DESCRIPTION

The best way to proceed is to draw a schematic picture of the molecule. Some day you will be able to do this directly on the graphics system, but for now pencil and paper will have to do.

Now choose a symbolic name for the molecule. The name may be up to four characters long.

Now assign each atom a unique name of up to four characters. This completes the definition of the molecule's nomenclature.

In order to uniquely describe the intra- and inter-molecular connections it is best to attempt to view the molecule as containing a linear chain of atoms from which all other atoms branch to form sidechains and rings. These atoms are placed in one of six categories:

1. MAINCHAIN
   atoms are a linear sequence of bonded atoms. *Mainchain* atoms should be chosen with the knowledge that **MOLASM** links subunits together by connecting the last atom of the previous mainchain with the first atom of the current mainchain. The order of atoms in the *mainchain* is therefore important and should remain consistent between molecules of the same type.
2. SIDECHAIN
   atoms are the remaining atoms which branch off the *mainchain* or other *sidechain* atoms.

A complication occurs when atoms which are present in the *mainchain* must be removed to make the intermolecular bond. You may have to redefine some *mainchain* atoms as:

3. INITIATORS
   are atoms to be removed from the beginning of the *mainchain*.
4. TERMINATORS
   are atoms to be removed from the end of the *mainchain*.
5. SOLVENTS
   This category is for structures containing atoms with no covalent bonds. These structures would be invisible in the MMS line drawing display. A typical example of this situation is the case of water where only the oxygen position is known. An atom of this type is displayed with a tetrahedral symbol to make the atom position visible.
6. IONS
   This category performs the same function as the *solvent* category, but a different symbol is used. Two intersecting octagons are centered around the atom position for this type of display.

INPUT FILE CONVENTIONS

Each line of the input text file has a keyword at the beginning which defines the meaning of the rest of the line. Most lines contain a sequence of atom names indicating the order in which the atoms of that type are connected. Atom names should be separated with tabs or spaces. Embedded spaces in atom names can be included by surrounding the desired characters with double quotes. Input may be in upper or lower case. All names are converted to upper case for internal use by this program. Lines must appear in the same order as their descriptions below.

REMARK
: (optional, but encouraged) is used for comments and is ignored by *newmol*. As many as desired may be included.

RESIDU
: defines a symbolic name of up to four characters for the molecule. A file with this name (converted to upper case) will be created in the current working directory.

INIT
: (optional) defines *initiator* atoms that precede the *mainchain*. If more than one line is necessary to define the *initiator* atoms, the last atom of the previous line is connected to the first atom of the new line. No rings are allowed in the *initiator* atom list.

MAIN
: defines the atoms of the *mainchain*. If more than one line is required to define the *mainchain* atoms, the last atom of the previous line will be connected to the first atom on the new line. No rings are allowed in the mainchain.

SIDE
: defines the branches and rings off the *mainchain* or other *sidechain* atoms. If the first atom on a line is a *mainchain* or *sidechain* atom that has already been defined, the rest of the atoms on the line form a chain starting at the first atom. If the first atom has not been previously defined, then the line is considered a continuation of the previous line.

TERM
: (optional) defines the atoms at the end of the *mainchain* in the *terminator* region. The first atom here is bonded to the last atom of the *mainchain*. The same rules apply here as for the *initiator* atoms.

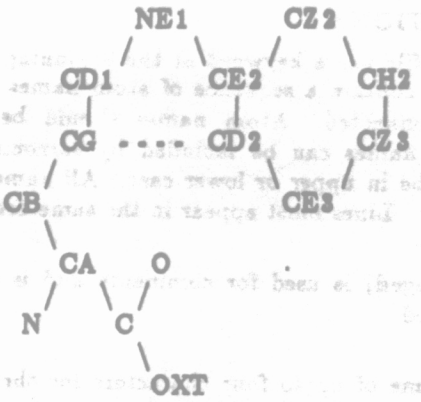
SOLVENT
: (optional) defines atoms to be displayed with the MMS solvent symbol.

ION
: (optional) defines atoms to be displayed with the MMS ion symbol.

ATOM or HETATM
: (optional) Brookhaven Protein Data Bank records which define coordinates for this structure. Not required unless you wish to view this database directly with the MMS.

EXAMPLE 1

The first example is of the amino acid tryptophan. This molecule is fairly easy to generate a description for since it has a clearly and commonly defined mainchain and sidechain. We choose the name "TRP" for this molecule, and label the atoms as:



Now determine the category for each atom. The *mainchain* atoms are N, CA, and C. Since the OXT atom is removed when this amino acid is linked to another the OXT is a *terminator*. All other atoms are *sidechain* atoms. The input file would contain the following lines:

```
residu  trp  1
main    n ca c
side    ca cb cg cd1 ne1 ce2 cz2 ch2 cz3 ce3 cd2 cg
side    cd2 ce2
side    c o
term    oxt
atom     1 n   trp   1     0.000   0.000   0.000  0.00  0.00
atom     2 ca  trp   1     1.450   0.000   0.000  0.00  0.00
atom     3 cb  trp   1     2.030  -0.830  -1.160  0.00  0.00
atom     4 cg  trp   1     1.490  -2.240  -1.200  0.00  0.00
atom     5 cd1 trp   1     1.820  -3.200  -2.100  0.00  0.00
atom     6 ne1 trp   1     1.140  -4.360  -1.840  0.00  0.00
atom     7 ce2 trp   1     0.340  -4.170  -0.750  0.00  0.00
atom     8 cz2 trp   1    -0.540  -5.040  -0.100  0.00  0.00
atom     9 ch2 trp   1    -1.220  -4.560   0.990  0.00  0.00
atom    10 cz3 trp   1    -1.020  -3.240   1.410  0.00  0.00
atom    11 ce3 trp   1    -0.160  -2.370   0.780  0.00  0.00
atom    12 cd2 trp   1     0.550  -2.810  -0.330  0.00  0.00
atom    13 c   trp   1     2.020   1.410   0.000  0.00  0.00
atom    14 o   trp   1     1.280   2.390   0.000  0.00  0.00
atom    15 oxt trp   1     3.350   1.490   0.000  0.00  0.00
```

Note that the order of the atoms in the sidechain ring was only one of many ways to describe this structure. We could have chosen:

```
side ca cb cg cd1 ne1 ce2 cd2 ce3 cz3 ch2 cz2 ce2
side cg cd2
```

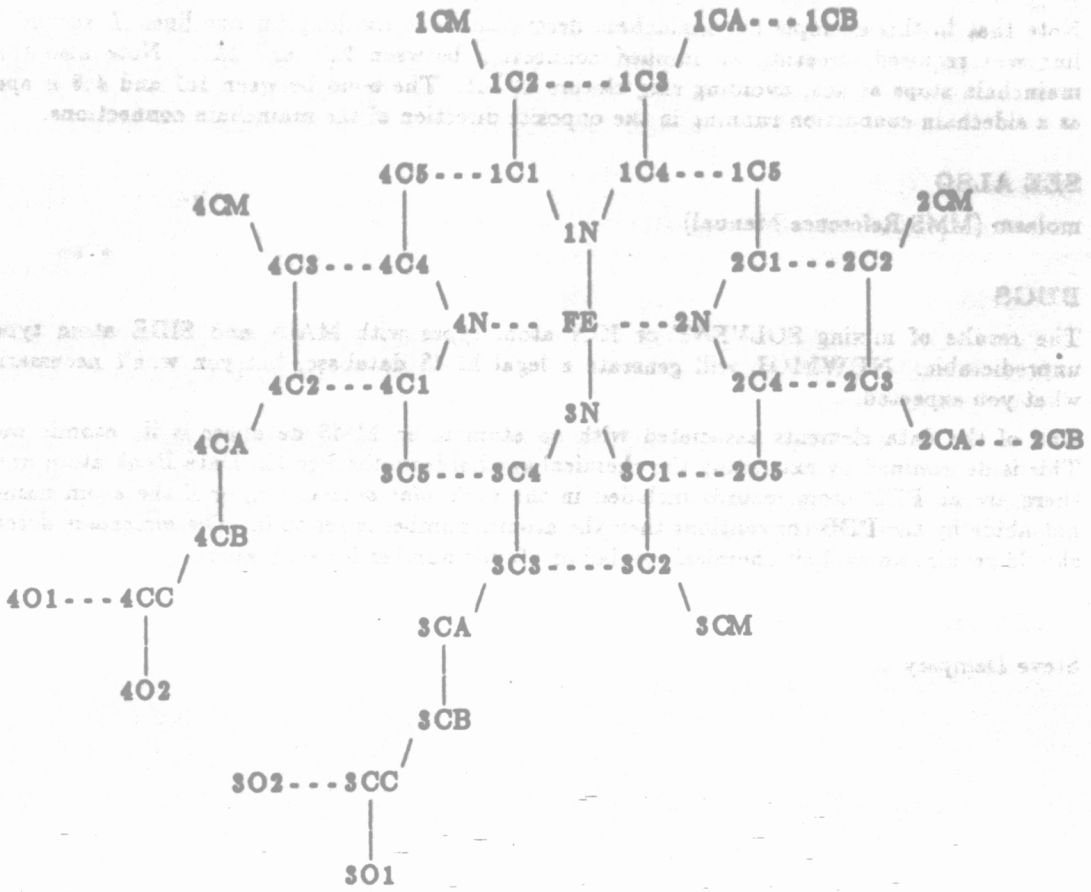
or

```
side ca cb cg cd2 ce2 ne1 cd1 cg
side ce2 cz2 ch2 cz3 ce3 cd2
```

as well. The order in which the sidechain atoms are traced is immaterial as long as all of the desired bonds are indicated.

EXAMPLE 2

For the second example we use a heme molecule to illustrate a case where the structure has no definite mainchain/sidechain configuration.



In a case such as this, one must choose an arbitrary sequence of atoms to make up the mainchain. Any sequence is valid as long as you don't attempt to close rings in the mainchain. We will choose the iron atom (FE) as the first atom and create the following input:

```
residu heme
main    fe 1n 1c1 1c2 1c3 1c4 1c5 2c1 2c2 2c3 2c4 2c5
main    3c1 3c2 3c3 3c4 3c5 4c1 4c2 4c3 4c4 4c5
side    1c1 4c5
side    1c2 1cm
side    1c3 1ca 1cb
side    1c4 1n
side    2c1 2n fe
side    2c2 2cm
side    2c3 2ca 2cb
side    2c4 2n
side    3c1 3n fe
side    3c2 3cm
side    3c3 3ca 3cb 3cc 3o1
side    3cc 3o2
side    3c4 3n
side    4c1 4n fe
side    4c2 4ca 4cb 4cc 4o1
side    4cc 4o2
side    4c3 4cm
side    4c4 4n
```

Note that in this example the mainchain description was too long for one line. A second 'main' line was required, creating an implied connection between 2C5 and 3C1. Note also that the mainchain stops at 4c5, avoiding ring closure at 1c1. The bond between 1c1 and 4c5 is specified as a sidechain connection running in the opposite direction of the mainchain connections.

SEE ALSO

molasm (MMS Reference Manual)

BUGS

The results of mixing SOLVENT or ION atom types with MAIN and SIDE atom types are unpredictable. NEWMOL will generate a legal MMS database, but you won't necessarily see what you expected.

One of the data elements associated with an atom in an MMS database is its atomic number. This is determined by extracting the chemical symbol from the Protein Data Bank atom name. If there are no PDB atom records included in the *molecular description*, or if the atom name does not abide by the PDB conventions then the atomic number is set to 0. The *molecular description* should require an explicit chemical symbol or atomic number for each atom.

AUTHOR

Steve Dempsey

NAME

molasm -- assemble macromolecular databases for MMS

SYNOPSIS

molasm [-i directory] input [output]

DESCRIPTION

MOLASM (MOLecular ASseMbler) uses information from your input file to select database templates which are linked together to form a larger database. Atomic coordinates and sequence identifications from the templates are then replaced with values from the input file.

If the optional argument -i is specified, then it must be followed by the pathname of a directory. When MOLASM is searching for templates, it will search this directory before the standard directory. This allows users to maintain private collections of molecular templates.

The output file name is optional. If it is not specified the output database will be placed in a file called *pic* in the current working directory.

INPUT FILE FORMAT

The input file is a standard UNIX ascii text file containing Brookhaven Protein Data Bank format records. *Molasm* actively processes ATOM, HETATM, TER, and SSBOND records. All other are tolerated and ignored. MOLASM will also accept coordinate records using the format of Wayne Hendrickson's refinement program PROLSQ.

COORDINATE SYSTEM CONVERSION

PDB coordinates are always defined in a cartesian angstrom system. MOLASM multiplies the coordinates by 100 and rounds them to integers. Therefore, the maximum resolution of an MMS database is 0.01 angstroms.

RULES TO REMEMBER

(1) The input file may be in either upper or lower case. MOLASM converts all input to upper case for internal use.

(2) Subunits for which no standard currently exists will be ignored.

(3) If the first atom of the mainchain of a subunit has no coordinate record, a fatal error occurs. Otherwise incomplete subunits are included in the output database with the missing atoms suppressed.

STANDARD TEMPLATES

The following molecules are provided with the MMS distribution. These structures were provided by protein crystallographers, so you won't find any hydrogens.

ALA	alanine
ARG	arginine
ASN	asparagine
ASP	aspartic acid
CYS	cysteine
GLN	glutamine
GLU	glutamic acid
GLY	glycine

HEM	heme group
HIS	histidine
HOH	the oxygen of water displayed as an MMS solvent symbol
ILE	isoleucine
LEU	leucine
LYS	lysine
MET	methionine
MTX	methotrexate
NAD	nicotinamide adenine dinucleotide
NDP	nicotinamide adenine dinucleotide phosphate
PHE	phenylalanine
PRO	proline
SER	serine
THR	threonine
TRP	tryptophan
TYR	tyrosine
VAL	valine
WAT	the oxygen of water displayed as an MMS solvent symbol

FILES

/usr/local/lib/mms/templates
directory of standard molecular subunit databases

pic default output filename

SEE ALSO

newmol (MMS REFERENCE MANUAL)

AUTHOR

Steve Dempsey

NAME

kmolasm -- assemble macromolecular databases for MMS using Kraut format data

SYNOPSIS

kmolasm [-b] [-i directory] input [output]

DESCRIPTION

KMOLASM (Kraut MOLecular ASseMbler) is a local (UCSD) version of the MMS molecular database assembler. This program will not be supported in the future. Sites outside of UCSD should not even consider using it. Use the program MOLASM instead.

KMOLASM uses information from your input file to select database templates which are linked together to form a larger database. Atomic coordinates and sequence identifications from the templates are then replaced with values from the input file. Standard templates currently exist for the common amino acids, and many miscellaneous cofactors. The current list may be examined by listing the contents of the directory *lusr/local/lib/mms/templates*. If your favorite structure isn't included consult the document on the program NEWMOL for instructions on creating new molecules.

If the optional flag -b is specified, the rules for linking subunits together are modified to allow subunits with noncontiguous sequence numbers to be bonded together. Structures whose sequence numbering is designed to show deletions from homologous molecules will be displayed properly only if this flag is used.

If the optional argument -i is specified, then it must be followed by the pathname of a directory. When KMOLASM is searching for standard subunits, It will search this directory before the standard directory. This allows users to maintain private collections of molecular databases.

The output file name is optional. If it is not specified the output database will be placed in a file called *pic* in the current working directory.

INPUT FILE FORMAT

The input file is a standard UNIX ascii text file with records no longer than 80 characters, separated by newlines. The function of a record is determined by the first six characters. The rest of a record contains formated fields whose contents are peculiar to each record type. What follows is a description of each of the record types recognised by KMOLASM. The number in brackets (< >) indicates the column where the field starts. The next symbol indicates the field type, where:

F means a floating value
A means a left justified character string
I means a right justified integer value

The number after one of these symbols is the maximum field width. Someday we'll rid ourselves of the computer stone age and use free format input, but until then we have to remain compatible with old IBM card decks laying around. In any case, most of these records are generated by other programs, so you shouldn't have to spend much time counting columns on your terminal.

CELL

specifies the unit cell size and shape. This must be the **FIRST** record in the file.

< 01> A6 - 'CELL '
< 14> F7 - length of 'a' cell axis in angstroms.
< 21> F7 - length of 'b'.
< 28> F7 - length of 'c'.
< 35> F9 - interaxial angle alpha.
< 44> F9 - beta
< 53> F9 - gamma.

GRID

specifies the number of grid units along each unit cell axis. This record must be the **SECOND** record in the file.

< 01> A6 - 'GRID '
< 14> I4 - numbers of grid units along 'a' axis.
< 18> I4 - same for 'b' axis.
< 22> I4 - same for 'c' axis.

RESIDU

this record associates a sequence number with a particular standard subunit name. **KMOLASM** uses this name to search for a file that contains the subunit database.

< 01> A6 - 'RESIDU'
< 09> A4 - subunit name
< 13> I4 - sequence number
< 17> A1 - sequence insertion code (optional)
< 19> A1 - chain identifier (optional)

ATOMG

this record contains the atom type, position, isotropic temperature factor, atom name, sequence number, insertion code, and chain identifier. The sequence number/insertion code/chain identifier combination is used to relate a set of ATOMG records to a RESIDU record.

< 01> A6 - 'ATOMG '
< 08> A6 - atom type (chemical symbol)
< 14> F8 - X coordinate in grid units
< 22> F8 - Y coordinate
< 30> F8 - Z coordinate
< 38> F6 - temperature factor
< 44> A4 - atom name
< 48> I4 - sequence number
< 52> A1 - insertion code (optional)
< 54> A1 - chain identifier (optional)

SOLVNT

this record is used when a single atom subunit needs to be displayed (i.e., a water molecule without hydrogens). This is not possible with a normal subunit database since MMS displays only bonds between atoms. This record puts an entry into the database which will force MMS to display a small tetrahedral figure around the position specified on the SOLVNT record.

< 01> A6 - 'SOLVNT'
< 08> A6 - atom type (chemical symbol)
< 14> F8 - X coordinate in grid units
< 22> F8 - Y coordinate
< 30> F8 - Z coordinate
< 38> F6 - isotropic temperature factor
< 44> A4 - atom name
< 48> I4 - sequence number
< 54> A1 - chain identifier (optional)

ION this record performs the same function as the SOLVNT record, but draws a small sphere instead of a tetrahedral figure.

< 01> A6 - 'ION '
< 08> A6 - atom type (chemical symbol)
< 14> F8 - X coordinate in grid units
< 22> F8 - Y coordinate
< 30> F8 - Z coordinate
< 38> F6 - isotropic temperature factor
< 44> A4 - atom name
< 48> I4 - sequence number
< 54> A1 - chain identifier (optional)

BREAK

this record causes a break in the mainchain of the molecule. The break occurs between the subunits specified by the last and next RESIDU records encountered in the input file. This record should be used when two subunits with contiguous sequence numbers should not be pictured as covalently bound together.

< 01> A6 - 'BREAK '

BRIDGE

this record will cause a line to be drawn between the two atoms specified on it. It was designed to allow MMS to display non-standard inter-residue connections such as disulphide bridges and hydrogen bonds.

< 01> A6 - 'BRIDGE'
< 08> A4 - name of first atom
< 13> I4 - residue number of first atom
< 17> A1 - insertion code (optional)
< 19> A1 - chain identifier of first atom (optional)
< 22> A4 - name of second atom
< 27> I4 - residue number of second atom
< 31> A1 - insertion code (optional)
< 33> A1 - chain identifier of second atom (optional)

COORDINATE SYSTEM CONVERSION

KMOLASM converts the crystallographic grid coordinates of the input to cartesian angstroms, multiplies the results by 100, and rounds them to integers. Therefore, the maximum resolution of an MMS database is 0.01 angstroms. The cartesian coordinate system is generated from the crystal system as follows:

Given crystal axes a,b,c:

X = a.
Z = a cross b.
Y = a cross Z.

RULES TO REMEMBER

1. The input file may be in either upper or lower case. **KMOLASM** converts all input to upper case for internal use.
2. Any input record that doesn't match one of the above possibilities will be ignored.
3. ATOMG and RESIDU records must be sorted by sequence number into accending order. Failure to do so will usually result in **KMOLASM** complaining that it can't find RESIDU or ATOMG records. However, ATOMG records may appear in any order within a subunit.
4. SOLVNT records may appear anywhere after the GRID record.
5. Breaks in the mainchain will be introduced whenever there is a change in the chain identifier, a BREAK record appears between 2 RESIDU records, or the sequence numbers are not contiguous. If the *-b* flag is specified at run time then the sequence numbers are not checked for continuity. Otherwise, subunits are assumed to be bonded together.
6. Subunits identified by a RESIDU record but without ATOMG records will cause a fatal error.
7. ATOMG records which are not preceded by the corresponding RESIDU record will cause a fatal error.
8. Subunits for which no standard currently exists will be ignored.
9. If the first atom of the mainchain of a subunit has no ATOMG record, a fatal error occurs. Otherwise incomplete subunits are included in the output database with the missing atoms suppressed.

FILES

/usr/local/lib/mms/templates
directory of standard molecular subunit databases

pic default output filename

SEE ALSO

newmol (MMS REFERENCE MANUAL)

AUTHOR

Steve Dempsey

NAME

contour – generate an MMS database containing electron density contours

SYNOPSIS

contour function [output]

DESCRIPTION

CONTOUR is a program which creates an MMS database that contains three dimensional contours of a subset of the sampled function contained in the file specified as the argument 'function'. If the output name is omitted the database will be placed in the user's current working directory under the name *con.out*. The contours are generated on the three planes parallel to the axes of the function's coordinate system.

USAGE

The unit cell parameters and layout of the input map will be listed, followed by a prompt:

enter origin of space to be contoured (zyx order)

Do exactly what it says, placing a space, comma, or tab after each number. The next thing you see is:

enter no. of points along each axis

Enter numbers as before, but keep in mind that a maximum of 30 points are allowed along any axis. If you don't keep it in mind, the program will let you know in no uncertain terms. It will also check to see that the values you entered are valid for the current input. Self explanatory nasty messages will follow if you goof, but the program is very forgiving and will let you make another attempt.

The next prompt is:

enter downhill blip length and density scale factor

The blips are those little tails that appear on contours to indicate the direction of lower density. The length is expected in angstroms. The default is zero, and the maximum is 0.1. The density scale factor defaults to 1.00. The numbers may be entered in any column as long as they are separated by a comma, tab, or space. The default values may be selected by hitting return without entering any numbers.

The final prompt is:

enter contour levels

The values should be entered on one line, with a comma, tab, or space after each. A maximum of eight contour levels are allowed. A return must follow the last level.

Assuming your input is reasonable, it will be listed on your terminal and you will be asked to verify it. A response beginning with a 'y' is considered an affirmative response. A 'q' followed by a return signifies final defeat and results in the termination of the program. Anything else (literally!) means you want to take another crack at it. This is a good time to vent any frustrations you may have accumulated. If you have entered everything correctly there is nothing left to do except sit back and watch. A message will appear as contouring is completed at each contour level.

CAUTIONS

Although CONTOUR can process a volume of up to 30 grid units on a side at 8 contour levels, the size of the generated database is dependent on the number of segments needed to draw the contours. It is quite possible for this program to generate a database which exceeds the maximum database size for MMS (approx. 128,000 bytes).

FUNCTION FILE FORMAT

The input file is a binary file containing a header followed by the function values. Function values are stored as signed 16-bit integers.

byte address	data
0-79	80 character ascii XRAY CELL record format: 'CELL',9x,3f7.3,3f9.5 specifying a, b, c, alpha, beta, gamma
80-85	x,y,z grid specs
86	number of points along X
88	origin of X
90	increment along X (usually 1)
92-97	same for Y
98-103	same for Z
104	scanning (summation) order for X
106	same for Y
108	same for Z (3 is fastest, from point to point; 2 is from line to line; 1 is slowest, from page to page)
110-EOF	density values in scanning order

AUTHOR

Steve Dempsey

NAME

chain – generate an MMS database of chained atoms

SYNOPSIS

chain < input [>] output

DESCRIPTION

Chain reads a file containing PDB atom coordinate records from the standard input. Chain will then generate an MMS database which will connect each atom position with a line in the order encountered. Gaps will be inserted in the chain when an input line is read with the word 'TER' on it. The database is written to the standard output unless a valid filename is given as an argument.

AUTHOR

Steve Dempsey

CHAPTER 5

Database Display Tools

This chapter documents the components of the UCSD Molecular Modeling System which are used to interactively view and manipulate images of molecular models. All of the graphics interaction is controlled by a single program called MMS.

NAME

mms toolbox – molecular modeling system display program

SYNOPSIS

mms

DESCRIPTION

Mms is the interactive graphics component of the UCSD Molecular Modeling System. You interact with the graphics system by manipulating various devices. The IRIS devices include:

(1) the terminal keyboard. Note that this is not necessarily the IRIS keyboard. If you log in and start MMS from an auxiliary ascii terminal then the terminal's keyboard will be used by the MMS.

(2) the mouse. The mouse is a device for controlling the two dimensional position of a point. The translation of the mouse is recorded as it rolls around on a surface. It is most frequently used to position a cursor on the graphics screen.

MMS is organised as a *toolbox,* from which you may select an assortment of *tools,* each of which performs a specific set of functions. You open the toolbox by starting the program. The available tools are presented in a menu on the left edge of the screen. A tool is selected by moving the mouse until the cursor is over the desired menu item, and then pressing the left mouse button. The upper left corner of the screen will contain the name of the current tool. The toolbox menu will be replaced with the appropriate menu for the selected tool. Items are selected from the tool menu in the same manner as from the toolbox menu. As a general rule, items in a tool's menu are drawn with a green background to indicate that the function associated with the item has been activated. Otherwise, the item is drawn with a red background.

Subsequent tools are selected by returning to the *toolbox.* You return to the toolbox by placing the cursor over the **TOOLBOX** icon at the bottom of the screen and pressing the left mouse button. The toolbox menu will reappear on the left hand side of the screen. When a new tool is selected the previous tool is placed into an area called the *tool table.*

The *tool table* appears across the bottom of the screen and contains the names of the five most recently used tools of the current session. Tools are selected from the tool table in the same manner as from the toolbox. The purpose of the tool table is to allow one to switch directly from one tool to another without going back to the toolbox. When the tool table is full the least recently used tool falls off the tool table and is placed back in the toolbox. Tools currently on the tool table will be draw in the toolbox menu with a green background. The rest will have a red background.

The current session is terminated by selecting the item called **END SESSION** from the toolbox menu. You will be asked to verify that you really want to quit. If you answer affirmatively you will then be asked if you wish to save any of the MMS databases from the current session.

AUTHOR

Steve Dempsey

NAME

MMS Atom Specification Syntax

SYNOPSIS

[*#model number*] [*/atom name*] [*:residue name*] [*;chain identifier*] [*%number*] [*,*]

DESCRIPTION

Many MMS tools perform functions which require you to specify a subset of the atoms from the current databases. A set of atoms is described by a string of characters called an *atom specification*. An atom specification consists of 4 basic parts, each of which is preceded by an identifying symbol.

1. '#' model number
   A model number is a decimal number in the range 1 to 10. Once a model number appears in an *atom specification*, it becomes the default model number for the rest of the command line.
2. '/' atom name
   An atom name is a string of up to 4 non-blank characters. Double quotes surrounding the name can be used to include embedded blanks or the reserved characters used in *atom specifications*.
3. ':' residue name or number
   A name is a symbol of up to four characters. A number may be immediately followed by a single letter to indicate an insertion code.
4. ';' chain identifier
   A chain identifier is a single character.

Any or all of the parts of an *atom specification* may be missing. When a part is missing, all atoms are treated as if they matched that part. For instance, when the model number is missing the command applies to all models. No specification implies all atoms of all models under MMS control. Note that blanks within atom specifications are optional.

EXAMPLES

A model number specifies all atoms in one model.

#1 selects all of the atoms of model 1.

An atom name specifies all atoms with that name.

/cb selects all atoms with the name "cb".

A dash placed after an atom name specifies the atoms on all branches that start with the named atom.

/cb- selects all amino acid sidechains.

A residue name specifies all atoms in the named residues.

:his selects all atoms in histidines.

A residue number specifies all atoms in residues with the indicated sequence number.

:10a selects all atoms in residues numbered 10a.

Two residue numbers separated by a dash specify all atoms belonging to an inclusive range of residues.

:10-20 selects all atoms in residues 10 through 20.

A chain identifier specifies all atoms with that chain code.

;s selects all atoms with the chain code 's';

Model numbers, atom names, residue designations, and chain codes may be combined to produce more restricted atom specifications.

#1/ca selects all alpha carbons in model 1.

#1:10 selects all atoms in residue 10 of model 1.

#1:10-20 selects all atoms in residues 10 through 20 of model 1.

#1:his selects all atoms in the histidines of model 1.

:his;x selects all histidine atoms in chains labeled 'x'.

/ca:10-20 selects all alpha carbons in residues 10 through 20 of all models.

#1/cb-:10-20 selects all sidechains in residues 10 through 20 of model 1.

Up to six *atom specifications*, separated by commas, may be included in one command line.

#3/ca, /cb, #1:10-20, #2/cb- selects all alpha and beta carbons of model 3, residues 10 through 20 of model 1, and all sidechains of model 2.

A modulo operator is provided by the percent sign.

/ca%10 selects every tenth alpha carbon.

NAME

models – MMS database selection tool

DESCRIPTION

Models is the MMS tool which controls the set of MMS databases for the current session. When this tool is selected the list of current databases will be displayed in the center of the screen. Next to each filename will be a count of the number of vectors used to draw the current image of the model and the model number assigned to the database. Note that the MMS always works with a copy of the file. The actual database file will never be modified by the MMS.

MENU ITEMS

ADD

This item is selected to add another MMS database to the current set. Up to ten models may be in use at any one time. You will be asked to enter the filename of the new model. It will be assigned to the lowest available model number.

REPLACE

This item is selected to delete a model and replace it with another such that the new model is in the same frame of reference as the one it replaces. The model to be replaced is selected by moving the cursor into its box in the center of the screen and pressing the middle mouse button. You will be given the option of saving the internal version of the database before it is deleted from the MMS session.

DELETE

This item is selected to remove a model from the current MMS session. The model to be deleted is selected by moving the cursor into its box in the center of the screen and pressing the middle mouse button. You will be given the option of saving the internal version of the database before it is deleted from the MMS session.

SAVE

This item is selected to save the internal version of an MMS database in a file. The model to be saved is selected by moving the cursor into its box in the center of the screen and pressing the middle mouse button, whereupon you will be asked to enter a filename. If the file exists you will be given the option of overwriting it.

NOTES

Any of the operations initiated by selecting the menu items may be aborted by entering a null filename (*i.e.*, just hitting the return key) when a filename is requested.

NAME

view – MMS scene orientation and projection tool

DESCRIPTION

View is the MMS tool which allows you to manipulate the orientation of the molecular models displayed in the center of the screen. It also controls the type of projection, choice of stereo viewing technique, depth cueing, and other functions related to how you view your models. Note that this tool operates on the entire set of models at once, so that all models remain fixed with respect to one another. Other tools are used to move one model relative to another.

MENU ITEMS

The first seven menu items are selected to attach the cursor movement to various parameters which control the orientation and projection of the model scene. The cursor, via the mouse, can be thought of as an extension of your finger. The cursor is used to turn an imaginary thumbwheel which alters the value of the attached parameter. Your finger is placed on the thumbwheel by pressing and holding down the middle mouse button. The value will not change unless the middle mouse button is held down. An additional feature of the thumbwheel is that it is mounted on a frictionless bearing. If the thumbwheel is moving when your finger is lifted, it will continue to spin until you stop it by putting your finger down again.

These items are mutually exclusive. Only one is active at a time. The active item is drawn with a green background, while the others will have a red background. When an item is selected the cursor shape will change to indicate which direction (horizontal, vertical, or both) is used to alter the desired parameter.

XY ROTATE

Horizontal movement of the cursor is attached to rotation of the model scene around the laboratory vertical (Y) axis. Vertical movement of the cursor is attached to rotation around the laboratory horizontal (X) axis. A model's center of rotation is determined by averaging the coordinates of its displayed atoms. The origin of rotation for the entire scene is determined by averaging the centers of rotation from each model.

XY TRAN

The models in the scene are translated along the laboratory X and Y axes in synchrony with the cursor movement.

Z ROTATE

Horizontal movement of the cursor rotates the scene around the laboratory Z axis, an axis normal to the display screen.

Z TRAN

Vertical movement of the cursor translates the models along the laboratory Z axis.

HITHER

Vertical movement of the cursor translates the hither clipping plane along the Z axis. The hither plane is limited to the region between the yon clipping plane and a distance of one angstrom from the observer.

YON

Vertical movement of the cursor translates the yon clipping plane along the Z axis. The yon plane is not allowed to cross in front of the hither clipping plane.

VIEWANGLE / MAGNIFICATION

When a perspective projection is selected (see below) this item is labeled **VIEWANGLE**. Horisontal movement of the cursor then changes the perspective viewing angle. This is analogous to changing the focal length of a camera lens. When an orthographic projection is selected this item is labeled **MAGNIFICATION**. Horisontal movement of the cursor changes the scale of the image.

The next two items select the type of viewing projection.

PERSPECTIVE

ORTHOGRAPHIC

The next three items control various types of stereo displays.

MONO

Stereo is disabled when this item is selected.

PLZT STEREO

This item selects a mode where the left and right views are alternated on the screen. The assumption here is that some sort of shutter device is synchronised to the switching views. We originally used a Stereo-Optics PLZT shutter system, but will soon be installing a Tektronix Liquid Crystal Shutter system.

SPLIT STEREO

This item selects a mode where the scene area is split in half, with the left stereo image drawn on the left side and the right stereo image drawn on the right side.

The remaining items perform micellaneous functions.

VISUAL AID

When this item is selected the right side of the screen displays an orthographic view of the scene looking down on the viewing (Z) axis. The purpose of this display is to show the positions of the viewer and the hither and yon clipping planes with respect to the models. If the current projection is perspective, the viewing angle and the observers position are depicted. When an orthographic projection is in effect the scale factor is shown.

CLIP LOCK

When this item is selected the clipping planes will move when the models translate along the Z axis. This is most often used to preserve the depth cueing effect while changing the apparent size of the models. The clipping planes are normally fixed and do not move when the models are translated along the Z axis.

DEPTH CUE

This item enables a mode where the intensity of a model diminishes with its distance from the observer. The intensity gradient ranges from brightest at the hither clipping plane to dimmest at the yon clipping plane. When this item is enabled the hither and yon clipping planes are automatically positioned around the models, producing the maximum depth cueing effect across the entire set of models. The clipping planes may then be moved to alter the depth cueing effect.

TIMING

When this item is selected the approximate speed of the program in frames per second is displayed on the standard output every 100 frames.

RESET

This item restores certain values when it is selected. The scene is translated so that the center of rotation is in the center of the screen, 30 angstroms in front of the observer. The view angle is set to a default value, and the clipping planes are moved to extreme positions. This item is generally used when the models have disappeared off the edge of the visible universe.

NAME

logbook – MMS electronic logbook (under construction)

DESCRIPTION

Logbook is an MMS tool which will have the ability to record and playback an MMS session. The functions of this tool are modeled after a tape recorder.

MENU ITEMS

RECORD

When this item is selected you will be asked to enter a filename. It will be used to create a file in which the session will be recorded. Recording begins when you hit return.

PLAY

When this item is selected you will be asked to enter the name of a file containing a previously recorded MMS session. Upon hitting return MMS will be driven from the contents of the file instead of the mouse and keyboard.

STOP

This item is selected to stop RECORD and PLAY mode. Of course, you can only stop RECORD mode. The selection of STOP is the last operation recorded. PLAY mode ends when this last cursor motion is read from the file. Control of the MMS is then returned to the mouse and keyboard.

NOTES

The only reliable way to use this tool at the moment is to begin recording or playback immediately after MMS is started. This tool does not know the context of the program when it begins recording. Only the cursor motions and button changes are recorded, not the effects they have. Suppose you begin recording, enable a feature, and then stop recording. During playback the cursor will move to the same location and select the same menu item, but this time the feature will be disabled.

BUGS

Keyboard input is not recorded.

NAME

rendezvous – MMS molecular model docking tool

DESCRIPTION

Rendezvous is the MMS tool which is used to move models relative to one another. A subset of the current models are designated to be moved while the rest remain fixed in the laboratory frame of reference.

MENU ITEMS

The first five items operate in the same manner as the similar functions of the view tool, but only affect the models which have been selected.

XY ROTATE
: Rotates the models around the laboratory X and Y axes.

Z ROTATE
: Rotates the models around the laboratory Z axis.

XY TRAN
: Translates the models along the laboratory X and Y axes.

Z TRAN
: Translates the models along the laboratory Z axis.

VISUAL AID
: Displays a view of the Z axis as in the VIEW tool.

OVERLAY
: This item is selected to overlay or superimpose the coordinate systems of certain models. The first model selected (see below) will remain fixed in the laboratory frame of reference. Each subsequent model that is selected will have its coordinate system overlayed onto that of the first model selected.

The last ten items are used to select models. When a model is selected the menu item will have a green background.

MODEL 1

MODEL 2

MODEL 3

MODEL 4

MODEL 5

MODEL 6

MODEL 7

MODEL 8

MODEL 9

MODEL 10

NAME

display edit – MMS display editing tool

DESCRIPTION

Display Edit is the MMS tool that determines which parts of an MMS database are displayed and labeled. Atoms are selected either by typing an *MMS Atom Specification*, or by placing the cursor on an atom and pressing the middle mouse button.

MENU ITEMS

The first five items edit the display.

DISPLAY
: This function is used to redisplay atoms which have been deleted. *MMS Atom Specifications* are required here. You can't hit an atom if you can't see it.

DELETE
: This function is used to delete atoms from the display. When an atom is deleted connections to its neighbors are erased. If atom A is connected to atom B which is connected to atom C, and atom B is deleted, then the lines from B to A and B to C are erased.

SHOW
: This function shows only the atoms specified, and deletes everything else. This is equivalent to deleting everything and then displaying the desired atoms.

BACKBONE
: This function shows only the atoms specified, and connects them with lines. This is equivalent to skipping everything and then displaying the desired atoms.

SKIP
: This function deletes atoms from the display but connects atoms that were attached to the skipped atom. Given the same example as described for DELETE above, the result would be the same except that a new line between atom A and atom C would be drawn. This feature is seldom used by itself, but its mechanism is used to implement the BACKBONE function.

The last four items control atom labels.

LABEL
: This function labels atoms with the atom name, residue number, and chain identifier (if any).

SLABEL
: This function generates a label consisting of the chemical symbol only.

RLABEL
: This function generates a label containing the residue name, residue number, and chain identifier (if any).

UNLABEL
: This function removes any of the above labels from the specified atoms.

NAME

color edit – MMS color editing tool

DESCRIPTION

Color Edit is the MMS tool that allows you to alter the color of selected parts of MMS databases. When this tool is selected a color palette appears on the right side of the screen. A color is selected by placing the cursor on the desired color and pressing the middle mouse button. Atoms are selected either by typing an *MMS Atom Specification*, or by placing the cursor on an atom and pressing the middle mouse button. When two connected atoms are different colors, the line between them will change color at its midpoint. Color information is recorded in the MMS database and will be retained if the database is saved to a disk file.

MENU ITEMS

BLINK

When this item is enabled a single color may be blinked. The color is selected by hitting an atom of the desired color or one of the colors in the color palette.

UNBLINK

When this item is selected the blinking color stop blinking.

NAME

model builder – MMS model building tool

DESCRIPTION

Model builder is the MMS tool which is used to change the shape of molecules.

MENU ITEMS

The first four menu items provide for rotation and translation of the entire set of models. They are identical in operation to the same items in the VIEW tool.

XY ROTATE

Z ROTATE

XY TRAN

Z TRAN

The next three items are used to define various types of internal transformations. When an item is enabled the cursor and middle mouse button are used to hit the desired bonds.

TWIST

This item enables the definition of a rotation around a bond to alter a dihedral angle. A symbol consisting of an arc will be drawn around the bond hit with the cursor.

BEND

This item enables the definition of a rotation that alters a bond angle. Two bonds with a common atom must be hit with the cursor. When the bond bend is defined a symbol consisting of an arc and the rotation axis will be drawn through the common atom.

STRETCH

This item enables the definition of a bond stretch. When the bond is hit with the cursor a symbol consisting of a segment with arrowheads at each end is displayed near and parallel to the bond.

The next four menu items are used to manipulate previously defined transformations.

ADJUST

When this item is enabled the cursor movement can be attached to a previously defined transformation by placing the cursor near the symbol of a transformation and pressing the middle mouse button. The color of the symbol will change from red to green. Only one transformation may be attached to the cursor at a time. Horizontal movement of the cursor with the middle mouse button pressed will change the value of the transformation.

RESET

When this item is enabled and a transformation symbol is hit with the cursor the value associated with the transformation will be set to zero.

DELETE

When this item is enabled and a transformation symbol is hit with the cursor the transformation will be removed.

FREEZE

When this item is enabled and a transformation symbol is hit with the cursor the coordinates of the atoms affected by the transformation are updated before the transformation is removed. This command modifies the information in the internal copy of the *MMS database*.

BUGS

When a bond rotation is defined, the atoms at one end of the bond remain fixed, while atoms at the other end rotate around the bond. The selection of the fixed and rotating ends is currently not under the control of the user. It is a function of the order in which the atoms are drawn, which is in turn a function of the structure of the *MMS database*. The next release of MMS will allow the user to specify the fixed and rotatings ends.

NAME

unit cell – manipulate a model's unit cell parameters

DESCRIPTION

Unit Cell is the MMS tool which controls the unit cell parameters and display of the unit cell of the MMS databases in the current session. This tool operates on one model at a time, as selected from the menu.

MENU ITEMS

The first three menu items are used to manipulate unit cell parameters.

NEW CELL
: This item is selected to change the unit cell parameters of the model selected from the menu. You will be prompted for the unit cell lengths and angles.

DISPLAY CELL
: When this item is selected the unit cell box for the currently enabled model is displayed with the model. The edges of the unit cell box are drawn in green, with the origin and the ends of the a, b, and c axes labeled with O , A , B , and C respectively.

LIST CELL
: When this item is selected the unit cell parameters for the currently enabled model are displayed on the terminal screen.

CRYSTALLIZE
: Each time this item is selected one more layer of unit cells are added to the display, *i.e.,* from one unit cell to 3x3x3 to 5x5x5, *ad infinitum*. It is possible to generate a display containing literally millions of vectors with this function. This has the side effect of making the program run very slowly, reducing the response time from a fraction of a second to several minutes.

DISSOLVE
: Each time this item is selected one layer of unit cells are removed from the display. As noted above, if a large number of vectors are displayed the program may take a while to respond.

The remaining ten items are used to select the model upon which the above items will operate.

MODEL 1

MODEL 2

MODEL 3

MODEL 4

MODEL 5

MODEL 6

MODEL 7

MODEL 8

MODEL 9

MODEL 10

NAME

symmetry – manipulate the display of symmetry related models

DESCRIPTION

Symmetry is the MMS tool which controls the display of symmetry related copies of a model. The symmetry operations for the currently selected model are displayed in the upper right corner of the screen. The operations are colored red or green to indicate whether the symmetry related model is displayed. Symmetry related displays are controlled by placing the cursor on the desired operation and pressing the middle mouse button.

MENU ITEMS

LOAD SYMOPS

When this item is selected you will be asked to enter the name of a file containing the desired symmetry operations. The symmetry operations should be defined with the same syntax as used in the *International Tables of Crystallography*, except the *bar* symbol is replaced with a minus sign. Valid symmetry operations will be displayed in the upper right corner of the screen. A maximum of 50 symmetry operations are allowed.

The remaining ten items are used to select the model upon which this tool will operate.

MODEL 1

MODEL 2

MODEL 3

MODEL 4

MODEL 5

MODEL 6

MODEL 7

MODEL 8

MODEL 9

MODEL 10

NOTES

The application of symmetry operations to a model assumes that the proper unit cell parameters have been assigned with the **UNIT CELL** tool.

NAME

measurements – real-time distance and angle measurement

DESCRIPTION

Measurements is used to measure interatomic distances, bond angles, and torsion angles. Once a measurment is defined it remains active and is continuously updated. Thus they may be used in conjunction with the Rendezvous and Model Builder tools to monitor inter and intramolecular contacts while structures are moved. This tool can also be used to generate coordinate files.

MENU ITEMS

The first three items are used to define the type of measurement desired.

DISTANCE

> **This item enables the definition of a distance measurement. The cursor and middle mouse button are used to select the two atoms between which the distance will be measured. A dashed yellow line will be drawn between the atoms, with the distance in angstroms displayed at the center of the line.**

BOND ANGLE

> **This item enables the definition of a bond angle measurement. The cursor and middle mouse button are used to select the three atoms between which the angle will be measured. A dashed yellow line will be drawn between the atoms, with the angle in degrees displayed at the center atom.**

TORSION ANGLE

> **This item enables the definition of a torsion (dihedral) angle measurement. The cursor and middle mouse button are used to select the four atoms between which the angle will be measured. A dashed yellow line will be drawn between the atoms, with the angle in degrees displayed between the two middle atoms.**

The next item is used in conjunction with the previous three.

REMOVE

> **This item is used to remove a measurement. When selected the cursor changes to something resembling a pencil with an eraser on one end. To remove a measurement, place the eraser on the dashed yellow line and press the middle mouse button.**

The last two items are used to generate coordinate files. In both cases you will be asked for a model number in whose frame of reference the coordinates will be generated, a *MMS Atom Specification* to define the set of atoms for which coordinates will be generated, and for each model specified the name of a file to be created.

PDB COORDS

> **This item is selected to generate a coordinate file in the Brookhaven Protein Data Bank format.**

WH COORDS

> **This item is selected to generate a coordinate file in the format used by Wayne Hendrickson's refinement program *PROLSQ*.**

NAME

hardcopy – generate hardcopy output of the screen image

MENU ITEMS

PLOT

When this item is selected you will be asked to enter the name of a file into which plot data will be stored. The format of this file is the contents of an IRIS feedback buffer of the image in the scene viewport. At UCSD this file is plotted on the Chemistry department's laser printer with the command:

irisplot *file* **| rsh chemc plot -Tlaser**

PHOTOGRAPH

When this item is selected the screen image is set up to be photographed. The menu and tool table are erased, leaving only the models. The image remains in this mode until you press return on the keyboard. You then return to the MMS toolbox.

NAME

surface – manipulate the display of molecular surfaces

DESCRIPTION

Surface is the MMS tool which controls the calculation and display of various types of molecular surfaces. The surfaces are modeled with arrays of dots distributed over the surface of spheres. The dots will have the color of the atom with which they are associated.

Van der Waals surfaces are calculated as needed. The calculation of solvent accessible surfaces requires so much time that it is not a suitable feature for an interactive graphics program. Instead, this tool will read files containing the precalculated coordinates of the dots.

The right side of the screen will display the radius for each atom type. The default values for C, N, and O have been increased slightly to account for implicit hydrogens. The metal radii are the crystal ionic radii.

MENU ITEMS

NEW RADII

This item is selected to alter the default Van der Waals radii used in the surface calculations. You will be asked to enter the name of a file containing alternate radius values. Each line of the file should contain a chemical symbol and a radius in angstroms, separated by blanks or tabs. If no filename is entered the default values will be restored.

CALCULATE VDW

This item is selected to calculate and display the Van der Waals surface. You will be asked to enter the desired density of the dots and a *MMS atom specification* describing the set of atoms around which the surface will be generated. For each affected model, any surface generated from a precalculated file will be removed. Otherwise, each invocation of this item adds to the current Van der Waals surface display.

SURFACE FILE

This item is selected to read a file containing the coordinates of the dots of a surface. You will be asked to enter a filename and the number of the model with which the surface should be associated. The file should contain a Brookhaven Protein Data Bank **ATOM** or **HETATM** record for each atom in the surface, each of which is immediately followed by a dot count record (format *I5*) and then by one record for each dot. The format of a dot coordinate record is *3F10.4*, containing X, Y, and Z. Any Van der Waals surface associated with the model will first be removed. Otherwise, each invocation of this item adds to the current surface display.

DELETE

Selection of this item removes all surfaces.

VISIBLE

Selection of this item toggles the visibility of the surface.

NAME

Unix shell – gain access to a UNIX command interpreter

DESCRIPTION

Unix shell is selected to execute your default shell in order to allow you to run a UNIX command without having to terminate the current MMS session. When this tool is selected your shell prompt will appear on the terminal screen. To return to MMS, log out. You will return to the MMS toolbox.