RELEASE NOTES

MidasPlus Version 1.8

Computer Graphics Lab
Department of Pharmaceutical Chemistry
University of California
San Francisco, CA 94143-0446

These release notes apply to MidasPlus version 1.8. This document summarizes the enhancements to existing commands, new commands that have been added, and bugs that have been fixed since version 1.5. Known problems are also listed. Only changes are summarized here. For full information about a command see the MidasPlus User's Manual or the on-line help system.

1. General Enhancements

1.1. UNIX Command Line Interface

Midas has two new command line options, a **–d** *delegate_name* option to treat standard input and output as a delegate with the given name, and a **-s** *script* option that sources the given script once *midas* has finished initializing.

1.2. MIDAS databases are gone!

The binary formatted MIDAS databases that helped so much on PDP-11's but hinder us now are finally gone. *MidasPlus* on the Silicon Graphics IRIS can still read MIDAS databases, but can not generate them. On the *NeXT* workstation MIDAS databases are not supported at all.

1.3. Atom Specification

Color is now an atom property. For example:

color red /color=blue

will make every atom currently colored blue be red instead.

The PDB helix and sheet attributes are now available as atom properties too. For example:

color red /strand
color green /helix
color blue /!strand,!helix

will color the sheets red, the helices green, and the turns blue.

1.4. RGB Color Support

The way color is defined in MidasPlus has changed substantially in this release. Colors are no longer limited to 62 saturated colors (plus white, gray, and black), but rather the user can arbitrarily create any color he/she wishes by defining the red, green, and blue primary components that make up that color See the **colordef** command below.

1.5. Picking

MidasPlus now distinguishes between multiple picks and misses when a pick fails.

2. Enhanced Commands

2.1. color

The interpolation behavior of color ranges has changed to be in a counter-clockwise direction along a standard color wheel — blue–red and red–blue interpolate complementary sections of the color wheel. The **c** designation changes the interpolation direction to be clockwise. For example, the following two commands interpolate the same set of colors, but in opposite directions.

color blue-red #1

color red-blue,c #1

Color interpolation in done in the HLS (hue, lightness, and saturation) color space (see *Computer Graphics* by Foley, van Dam, Feiner and Hughes).

2.2. pdbrun

pdbrun can generate an unannotated PDB file by giving the **nouser** option. This is for programs that choke on unknown PDB records (*i.e.* programs that don't follow the specification).

pdbrun output now contains objects, distance monitors, and angle monitors. Also, pseudo-bonds that are generated by the **chain** command are denoted by the `CHAIN` keyword.

2.3. open

When a PDB file is **open**ed, the current directory is checked first, then the user's private PDB directory (*${HOME}/pdb/* on the IRIS, *${HOME}/Library/Mol/pdb/* on the *NeXT*), and then the system PDB directory is checked (*/usr/mol/pdb/* on the IRIS, */LocalLibrary/Mol/pdb/* on the *NeXT*).

2.4. help (*NeXT* workstations only)

On the *NeXT*, the MidasPlus **help** command with no arguments puts you in the Digital Librarian where you can search for the information you desire. Use the *Titles* button in the Librarian to list all of the available topics. If you wish to access the MidasHelp files directly with the Librarian (without starting up *MidasPlus* first), add */LocalLibrary/Midas/MidasHelp* as a target in the Librarian's bookshelf and select it as you would any other target.

By default, when you give the **help** command with an argument, MidasPlus interprets the argument as a topic name and displays the help file for that topic. If the topic isn't found, the Digital Librarian is invoked with the topic as the search string. If you want to always search for the topic in the Librarian (and not be limited to one word), put

devopt help_search on

in your private *.midasrc* file in your home directory, or change the default behavior for all users by putting the above command in */LocalLibrary/Midas/midas.rc*.

3. New Commands

3.1. colordef

Usage: **colordef** *color_name red green blue*

Usage: **colordef** *color_name existing_color_name*

colordef adds the given *color_name* to the list of color names that MIDAS recognizes. A color name is an arbitrary sequence of letters, digits, and underscores. A color name may be redefined at will. The *red*, *green*, and *blue* arguments must be floating point numbers between zero and one, inclusive.

By convention, *red*, *green*, *blue*, *cyan*, *yellow*, *magenta*, *white*, *gray*, *grey*, and *black* are predefined. And for backwards compatibility, the color names that correspond to the integers ranging from 0 to 65, inclusive, are predefined and may not be redefined.

Numerical Color Mapping

Color name	Equivalent color number	colordef value		
		red	green	blue
green	1	0.0	1.0	0.0
cyan	8	0.0	1.0	1.0
blue	16	0.0	0.0	1.0
magenta	24	1.0	0.0	1.0
red	32	1.0	0.0	0.0
yellow	48	1.0	1.0	0.0
white	0	1.0	1.0	1.0
black	64	0.0	0.0	0.0
gray/grey	65	0.5	0.5	0.5

Examples:

colordef activesite red

create a special color for the active site.

On the *NeXT*, the **colorpanel** color is constantly redefined to be the current color in the color panel when the Color Panel is active, but otherwise acts just like any normal color name.

3.2. colorrename

Usage: **colorrename** *color_name new_color_name*

colorrename replaces the given *color_name* with the *new_color_name*. The new color name is an arbitrary sequence of letters, digits, and underscores. This command is most useful on the *NeXT*, where one might color the active site with the **colorpanel** color, and then rename it to a different name to save it.

3.3. neon

Usage: **neon** *options*

The **neon** command produces a three dimensional ball and stick representation of the displayed molecule(s) with appropriate shadows. The current orientation and coloring is retained. This image is not interactive and takes anywhere from a minute to several minutes to produce. After the image is displayed, clicking the left mouse button returns to MidasPlus.

There are many options, which are detailed fully in the *neon* manual page included in Appendix 6 of the MidasPlus User's Manual. (The **neon** command is actually an alias that executes the **pdbrun** command and sends data to the **preneon** and **conic** programs.)

If you are interested in seeing some sample **neon** images created on a IRIS workstation, some good examples can be found in

> A.M. De Vos, M. Ultsch and A.A. Kossiakoff, ''Human Growth Hormone and Extracellular Domain of Its Receptor: Crystal Structure of the Complex'', *Science*, **255**, cover image and 306-312, (1992).

Dr. Thomas Hynes of the Protein Engineering Department at Genentech, Inc. wrote the **preneon** program and contributed it to the MidasPlus distribution.

4. New Utilities

4.1. dms

Dms replaces the **ms** command for producing molecular surfaces. **ms** suffered from many constraints (such as inability to handle chain ids, uncommon chemical elements, *etc.*) that **dms** does not have. **Dms** command line syntax is almost identical to that of **ms** (only alternate radii files are specified differently). Consult the **dms** manual page (Appendix 6) for further details.

Dms (which stands for *distributed MS*) can be installed so that it runs on multiple machines simultaneously for increased performance. For simplicity of installation the default version provided only runs on the local host. If you wish to compile and install the distributed version, consult the READ_ME file in /usr/local/src/midas/contrib/dms.

5. Bugs Fixed

- Fixed a problem with scaling in cross-eyed stereo.
- Labels (filenames, rotations, *etc.*) are displayed even if no atoms are displayed.
- If non-ASCII characters are found in a PDB file, then the file isn't really a PDB file.
- A chain break is inferred if the chain identifier of a new residue is different from the previous one.
- When resetting to the ''default'' position, molecules that were unopened at **savepos** time are now selected by default.
- Window redraws during help messages are now handled correctly.
- **pdbrun** output now numbers all atoms consecutively rather than restarting from one for each model.
- Objects associated with models are not saved in sessions.
- vdw surfaces are now recalculated after structure changes.
- Compressed object files are now read properly.
- An obscure bug in the virtual sphere object that caused molecules to sometimes collapse and disappear has been fixed.
- A bug that caused the **copy** command to hang if a title was not supplied on the copy command line has been fixed.
- The reading of certain unusual PDB files has been speeded up by an order of magnitude. The PDB files contained many identical non-standard residues whose connectivity could not be found in template files in the directories searched by MidasPlus. Now MidasPlus remembers when a template search has failed instead of re-searching each time the residue is encountered.

6. Known Problems

6.1. General Problems

- It is not possible to switch from one session to another without exiting MidasPlus.
- On color hardcopies generated with the **copy** command, bonds may cross in front of bonds that they should cross behind because bonds are not depth-sorted when generating 2-D PostScript.
- Picking does not work well when MidasPlus is in ''stereo walleye/crosseye'' mode. Users should pick on the right eye image only.
- It is not possible to have the atoms specified in the **watch** command checked against a subset of the remaining atoms.
- There can be no more than 16 distance, angle or rotation monitors. We hope to remove these limits entirely in a future release.
- Moving or resizing the MidasPlus window while MidasPlus is busy processing a command may leave the window in weird state. Moving or resizing the window again after the processing is finished will bring the window back to normal.
- Device option settings are saved in session files, even though they may cause the wrong

behavior on other workstations that are configured differently (*e.g.* ucsf_stereo).

- Without binary MIDAS databases, we have lost the capability to generate internal coordinates. We hope to have code that matches the X-PLOR internal coordinate format by the next release of MidasPlus.

6.2. IRIS Specific problems

- Under IRIX 4.0 or later, if the X window server is allowed to run for a long time it often develops erratic behavior, slowly uses more memory, and occasionally causes working applications to dump core during startup. Until SGI fixes this problem, a workaround is to arrange to have the X server killed when a user logs off the console. To do this, edit the file /usr/lib/X11/xdm/xdm-config and change the terminateServer property to True.
- Indigoes exhibit bizarre behavior when in stereo mode under IRIX versions up to at least 4.0.2. This behavior is known to be corrected in IRIX 4.0.5. If you have an Indigo and are running a release earlier than 4.0.5, contact your SGI representative and request IRIX 4.0.5 or later for your machine.
- The **neon** provided on your release tape may not work on releases of IRIX later that 4.0.2. If you are running a release later than 4.0.2 and find that **neon** does not work, there is a version of **neon** in /usr/local/bin (*neon.4.0.5*) that works for later releases of IRIX. You should rename the non-functional /usr/local/bin/neon (*e.g.* /usr/local/bin/neon.4.0.2) and rename *neon.4.0.5* to be **neon**.
- Under IRIX 4.0 or higher, the right mouse button no longer gives you a menu (in any application, including MIDAS). You need to hold down the ALT key while pressing the right mouse button to get the menu.

6.3. *NeXT* Specific problems

- On a color NeXTstation, **copy** files are shown in black and white even though all of the color information is present. This is due to a configuration bug in Display PostScript and should be fixed in Release 3.0 of NextStep (we hope).
- The mouse doesn't work properly unless the mouse ''Menu Button'' is enabled with the Preferences application.
- The **cartoon** application (and corresponding **ribbon** command in MIDAS) has not been implemented on *NeXT* workstations.

6.4. Reporting Problems

If you discover a bug in MidasPlus, we want to know about it! Please send us an electronic mail message addressed to **midas-bugs@cgl.ucsf.edu.** Please include as much detail as possible (for example the exact sequence of user commands that causes the problem and the name of the PDB file if this is relevant), and always make sure to include the version of MidasPlus you are running (see the **version** command). Although we can't promise to fix the problem, we will make every reasonable effort to do so.

7. User Contributed Software

We are now redistibuting software contributed from other sites running MidasPlus. Both the **dms** and **preneon** programs are ''user contributed software''. If you have developed programs explicitly for use with MidasPlus, we encourage you to contribute these for redistribution to other sites. MidasPlus ''delegate'' programs are especially encouraged (see Appendix 5 in the MidasPlus User's Manual for more information on delegates). Send e-mail to **midas-ideas@cgl.ucsf.edu.** if you have software you would like to contribute.