

MicroWorld

Version 1.1

Command Reference

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What is MicroWorld?

MicroWorld is a molecular display program, which calculates three dimensional models (Dreiding, Ball&Stick, Space Fill) from atomic space coordinates, e.g. from x-ray data. It features powerful functions which are, so far, quite rare with other programs of this kind (at least the ones under US\$ 500):

- * Antialiasing: smoothed edges of stick borders and mixed model lines.
- * Depth cueing: impression of three dimensional depth by a change of the brightness of the model parts with increasing distance to the observer.
- * Transparent space fill models.
- * Up to three different model types in one model.
- * Import of any background picture and optional cast of a model shadow onto it.
- * Alignment of the model to a point, a bond, or a plane.
- * Display of a color legend for element colors.
- * High quality printouts.
- * Mathematical coprocessor not necessarily needed.
- * Optimized for 256 colors, but also gives quite good results with 16 grays.

MicroWorld has been written in such a way, that also lower end machines, like a 16-color Mac LC without a math coprocessor, will produce model pictures in acceptable time and quality. Moreover, it runs equally well from system 6.07 to system 7. The only hardware requirements are a 68020 processor (or higher) and the presence of color QuickDraw.

If you use an extra large screen, you may have to assign more memory to the program (a total of about 1'200 kBytes or so) by using the "Get Info"-command of the finder.

Interactive movement of the molecule



translation cursor



rotation cursor

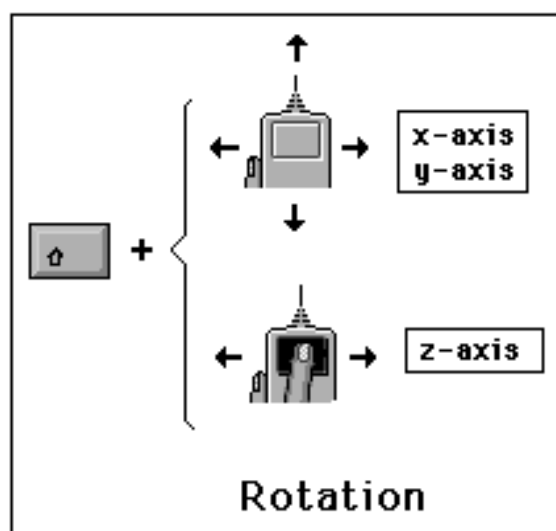
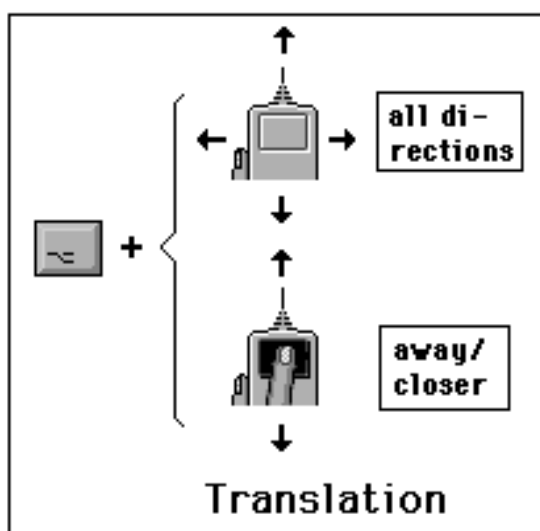
General:

The movement of a molecule on the screen is controlled by the simultaneous use of the mouse, a keyboard key and sometimes the mouse button. This corresponds to the way of moving objects on modern molecular modelling workstations.

Note: The orientation of the three rotational axes in space is shown in the "Positioning" menu (as menu graphics).

Note: The menu item "Interactive Movement" in the "Positioning" menu provides the picture below as an online help.

Rotation:	When pressing and holding the shift -key, the rotation cursor appears (see picture on top of page). Any subsequent mouse movement with the shift-key still depressed will rotate the molecule around its x- and y-axis. When the mouse button is pressed in addition to the shift-key, a horizontal mouse movement will cause a rotation around the z-axis.
Translation:	When pressing and holding the option -key, the translation cursor appears (see picture on top of page). Any subsequent mouse movement with the option-key still depressed will move (translate) the molecule in any direction on screen. When the mouse button is pressed in addition to the option-key, a vertical mouse movement will cause the molecule to move towards or away from the viewer.



Open ...
Save..
Save As...

MW-File



General:

MW-files contain all data required for the modelling of a molecule, such as its orientation in space, selections, labels, and so on. They are loaded much faster than external text files (ASCII) and are much more compact than MW-pictures (see MW Picture), since they don't additionally save a screen copy of the picture.

Examples of MW-files can be found in the "MW-files"- folder of the program disk.

Open ...	Opens the MW-file of a molecule, which is subsequently presented as wire frame model. The model settings remain unchanged.
Save...	Saves the actual position and all other relevant data of the displayed molecule as a MW-file. No copy of the screen picture is included (see MW-Pictures).
Save As...	Saves the molecule under a new name. In the appearing dialog window, a ".bin" is added to the end of the file name. However, the file can be given any name.

Import ...

General:

MicroWorld imports text-files (ASCII-files) from x-ray measurements, force field calculations, 3D-databases, or similar sources, provided they are in the format described below. Other formats have to be edited to the required format, e.g. by using a text program.

Note: If a scanner is used to read in the data, please make sure that it's software will properly distinguish the letter "O" from the number zero "0".

A text file in MicroWorld-format consists of a number of following lines:

label	x-coord	y-coord	z-coord
-------	---------	---------	---------	-----	-----

Example (more examples can be found in the "Import"-folder).

```
Cu128-0.123      2.435      -2.034
C1              0.345      -0.432-3.123
C2              0.143      1.453      2.341
...             ...             ...             ...
```

IMPORTANT: Above and below such a block of lines there should be no additional text or data. However, additional data to the right of the z-coordinate are tolerated. Data about atom connections are not required, since MicroWorld calculates these according to distance criteria.

The label of an atom may contain up to 7 characters and numbers, including brackets. The capitalization of the element symbols is not relevant. **The coordinates** may be any positive or negative numbers. All entries must be separated by spaces or tabs.

Opens an ASCII-file for import. In the case of "fractional" coordinates (coordinates relative to the crystallographic unit cell) a dialog window will appear and ask for further data (dimensions and angles of the unit cell). Otherwise, the atom connections will be calculated directly, and the molecule is presented in the wire frame model. <i>It is highly recommended to save the molecule immediately as a MW-file (see "Save").</i>

MW-Picture... **Open**
... **Save As**

MW-picture



General:

The contents of the working window can be saved as a standard picture file (PICT-format) which is accessible by almost every graphics application on the Mac. In addition to these standard picture data and invisible to other programs, this file also contains additional data of the represented molecule. This means that whenever a MW-picture is opened from within MicroWorld, it behaves just as if it would have been calculated a moment ago: after a mouse click, the underlying wire frame model appears which can then be moved and edited in the usual way.

Note: When a model containing a background picture is saved as MW-picture, the resulting file will not contain a separate copy of this background picture, rather a reference to its position (volume name, folder, file name) instead. Therefore, such a registered background picture should not be moved or renamed, should it be found again on opening the MW-picture.

Examples of MW-pictures can be found in the "Slide-Show"-folder of the program disk.

<p>Open: Opens a MW-picture. The size of the working window will adjust to the size of the picture, if possible. If the picture was saved in "full screen"-mode, the program will be switched into this mode. All model settings are updated.</p> <p>Save As: Saves the contents of the working window as a MW-picture. In the appearing dialog window, a ".pict" is added to the end of the file name. However, the file can be given any name. A MW- file can be read by almost all Macintosh graphics applications (PICT format).</p>
--

Background ...

General:

Background pictures sometimes dramatically enhance the visual impact of a shaded model on the viewer. Picture files from external paint programs, or from other sources, can be imported as background pictures, as long as they are in the PICT-format. Even MW-pictures can be used as background pictures, sometimes generating quite remarkable effects. If the "cast shadow"-option is on (see Model Settings), the model will cast a shadow on the background picture.

Examples of background pictures can be found in the "Backgrounds"-folder of the program disk.

Note: If the background picture uses quite a different color palette than the one MicroWorld uses, significant color shifts can occur. Recommendation: if you create your own picture, then open any already existing MW-picture from within your favourite paint program. The paint program will now contain the MicroWorld color palette. Erase the opened picture, paint your own background picture and save the resulting picture as PICT-file.

Note: When working with 16 grayscales, background pictures containing smooth color gradients should be avoided, since the limited amount of available grays will make them look quite coarse.

Note: The display of a background picture can be switched off temporarily by switching off the "Show background picture"-option of the "Model Settings"-dialog.

<p>Opens a background picture (PICT format). Its size is adjusted to the size of the working window, i.e. it is expanded or reduced to the right size. In the <i>wire frame</i> mode, only a message of the successful installation appears but the background will be visible during any subsequent model calculation. In the <i>color model</i> mode, the current model is recalculated using the new background.</p>

Page Setup ...

Print ...

Quit

General:

The best and, at the same time, least expensive method for the reproduction of color-computer graphics is to take a picture of the screen with a camera. As a general guideline, an aperture of 9.5 at 0.5 sec (tripod!) for an ISO 200 color slide film can be recommended; these values may vary with the brightness of the screen though and are best optimized by running a test series. To avoid distortions caused by the non-planar screen, the use of an objective with at least 80 mm is recommended.


Only today's most expensive color printers are able to print pictures in the quality of a color slide. Black and white graphics on the other hand can be printed out in much higher quality than a screen picture since, in this case, the quality of the color reproduction is guaranteed (black is black) and the resolution of the printer by far exceeds the one of the screen.

MicroWorld generates a high resolution printout, which is equally suited for QuickDraw- and PostScript-printers. It consists of a black and white graphics containing gray areas, which roughly corresponds to outline models (see "Outlines Only").

Note: Because of approximations in the printout of space fill models, these models should not be printed on a very large scale.

Page Setup ...	The standard print format dialog. It will also be displayed after every first print command after program start.
Print ...	Starts the printout of the current model as black and white graphics. In order to enable the printing of gray areas, "best" should be chosen for print quality; laser printers should be set to "color/grayscale".
Quit	Ends the program.

Copy
Partial Copy

copy cursor 

General:

Only the copy commands of the "Edit"-menu are active, i.e. picture data can be copied from the program to the clipboard but not vice versa.

Note: If the program, which receives the MicroWorld-graphics from the clipboard, does not have the same color palette as MicroWorld, significant color-shifts might occur. This is a problem of the receiving program and can not be influenced by MicroWorld.

Copy:	Copies the whole content of the working window to the clipboard. The picture data can be pasted into any document from there.
Partial Copy:	Copies a selected part of the screen to the clipboard. A copy-cursor (see picture at the top left of the page) appears, with which a rectangle around the desired area can be dragged. Its contents are copied to the clipboard, as soon as the mouse button is released.

Labels ... **Define/Use**
Clear All

General:

Atoms or a group of atoms are selected by clicking them with the mouse or alternatively by dragging a rectangle around them. Selected atoms are marked with a small circle. Already selected atoms become deselected by this process.

Selected atoms can be functionalized. They may carry a label, define a part of a mixed model, or define the basis for geometrical positioning or information.

"Labels" defines selected atoms as carriers of labels.

Note: The command "Show All Labels" (Model Menu) displays the labels of all atoms without selecting them.

Define/Use

Atoms without labels selected: The selected atoms receive a label. If there are already some labels defined, the new ones are added to these. The menu item is checked (if this is not already the case).

No atoms selected but already some labels defined : All defined labels disappear and the menu command is unchecked. By applying the command again, the labels reappear and the menu item is checked again.

Atoms already containing a label are selected : The label definition of these atoms is erased and the label disappears.

Clear All

All label definitions are erased and the labels disappear.

Mixed Model ... **Define/Use**
Invert
Clear All

General:

Atoms or a group of atoms are selected by clicking them with the mouse or alternatively by dragging a rectangle around them. Selected atoms are marked with a small circle. Already selected atoms become deselected by this process.

Selected atoms can be functionalized. They may carry a label, define a part of a mixed model, or define the basis for geometrical positioning or information.

The "Mixed Model"-command defines selected atoms as members of a partial-model within the main model. In this way e.g. parts of a space fill model can be defined as a Dreiding model. However, this mixed model part definition doesn't define any model types yet: these are assigned by the "Model"-menu (main model) and the "Model Settings" (partial model).

Define/Use	<p><u>Atoms without mixed model part definition selected:</u> The selected atoms are marked with a small rectangle. If some atoms already are defined as mixed model part, the new ones are added to them. The menu item is checked (if this is not already the case).</p> <p><u>No atoms selected but already some mixed model parts defined:</u> The mixed model part definitions are disabled temporarily and the menu item is unchecked. By applying the command again, the mixed model definitions reappear and the menu item is checked again</p> <p><u>Atoms already defined as mixed model parts are selected:</u> the mixed model part definitions of these atoms are erased.</p>
Invert	All atoms not defined as mixed model part are now defined as such and the definition of the others is erased.
Clear All	All mixed model part definitions are erased.

Edit Selection ... Invert
Clear All

General:

Atoms or a group of atoms are selected by clicking them with the mouse or alternatively by dragging a rectangle around them. Selected atoms are marked with a small circle. Already selected atoms become deselected by this process.

Apart from the above method of atom selection by the mouse, the selection of all atoms can be manipulated by following menu commands:

Invert:	All unselected atoms become selected and the selection of the others is erased.
Clear All	All atoms become deselected.

Geometrical Info

General:

Atoms or a group of atoms are selected by clicking them with the mouse or alternatively by dragging a rectangle around them. Selected atoms are marked with a small circle. Already selected atoms become deselected by this process.

The menu command "Geometrical Info" provides information about position, distance and angles of atoms, depending on how many atoms are currently selected. The values are given in Angstroms and degrees. The labels of the selected atoms are temporarily displayed until the information window is closed.

- 1 atom selected: The Cartesian coordinates of the selected atom are displayed.
- 2 atoms selected: The distance between the two selected atoms is displayed.
- 3 atoms selected: The three angles of the triangle defined by the selected atoms are displayed. Every angle is assigned to the corresponding centre.

Dreiding
Ball&Stick
SpaceFill

General:

These commands calculate one of the three main models from the wire frame model. Their appearance is influenced by the definition of the mixed model parts (see "Selection"-menu) and their assigned model types (see "Model Settings").

*Note: If either the mouse is clicked inside the working window, or an interactive movement is attempted, the calculated color model will immediately be replaced by the **wire frame** model since only this model type allows selections and interactive movements.*

Dreiding:	Calculates a model consisting of shaded sticks. Especially useful for complex structures.
Ball&Stick:	Calculates a model consisting of shaded balls and sticks.
SpaceFill:	Calculates a shaded space fill model.

Transp. SPF+Sticks

Transp. SPF+B&S

General:

In Space Fill models often parts of the molecule are hidden behind others. In order to compensate this, above commands will mix a transparent Dreiding or Ball&Stick model into the Space Fill model.

The amount of transparency can be adjusted within the "Model Settings"-dialog (Model-menu).

*Note: If either the mouse is clicked inside the contents of the working window, or an interactive movement is attempted, the calculated color model will immediately be replaced by the **wire frame** model, since only this model type allows selections and interactive movements.*

Transp. SPF+Sticks:	Calculates a Space Fill model and then overlays a transparent Dreiding model.
Transp. SPF+B&S:	Calculates a Space Fill model and then overlays a transparent Ball&Stick model.

Outlines Only
Show All Labels
Full Screen

General:

These options are switched on/off by selecting them repeatedly. Their menu items are checked accordingly.

Outlines Only:	Very fast model calculation in unshaded grayscales, but with depth cueing. Useful for first model overviews. Complex Ball&–Stick models often look less crowded in this model than in the corresponding color model.
Show All Labels:	The labels of all atoms are displayed. During an interactive movement of the molecule they are temporarily switched off.
Full Screen:	The working window is expanded to the whole screen, the menu bar disappears. However, when moving the cursor to the very top of the screen and pressing the mouse button there, the menu will appear as usual. The full screen mode might be the most convenient way to work with MicroWorld, and is indispensable when taking pictures of the screen.

Model Settings

Preferences icon



General:

In this dialog window, settings for several parts of the program can be defined. These are saved permanently by using the "SAVE"-button, or they are used temporarily by clicking the "OK"-button. If necessary, the model will be recalculated when the dialog window is closed.

Background Shadow:

A shadow of the model is cast onto the background (if it is not already black).

Show Background Picture:

The display of a background picture can be switched on/off by this option. If none is already opened so far, you will be requested to choose one.

Auto Darker On Pict:

Temporarily sets the option "Darker with Distance" (see below) whenever a background picture is present. This avoids unrealistic light situations on dark backgrounds.

Darker With Distance:

Depth Queing: Model becomes darker with distance. Black background, if no background picture present.

Brighter With Distance:

Depth Queing: Model becomes brighter with distance (dust effect). White background, if no background picture present.

Wire Frame DQ, Outlines DQ, Model DQ, Model-Labels DQ:

Switches the Depth Queing option (DQ; see above) of each model type and the model labels on and off. If switched off, no change in color brightness with distance occurs.

Color Legend:

Displays a moveable color legend, which reflects the color assignments of the current model (not visible in the wire frame model).

Transparency:

Amount of transparency of the transparent models. Range: 10-90%.

Mixed Model Parts Of...:

Assignment of a model type to the mixed model part of a main model (see "Selection"-menu). No such assignment is required for the Dreiding model since only lines are possible as part model type of this model.

Color Settings

Preferences icon



General:

This dialog allows the assignment of different colors to the elements. The colors themselves can not be edited.

These assignments are reflected in the optional color legend window (see "Model Settings").

The desired element symbols are entered into the text fields to the right of the color boxes. Old entries are replaced directly and without previous deleting by clicking their text field and entering the new text. While typing, the first letter of the element symbol is formatted to upper case, the second (if present) to lower case.

All element symbols, which occur in the model but are not defined in the Color Settings are assigned the color shown at "others".

Default: Resets all color assignments to their standard values.

Save: Saves the color assignments permanently in the preferences file, i.e. they will be active after every program start from then on.

OK: The color assignments will be used as long as the program is running.

Align

General:

This command aligns the molecule exactly along a defined axis or plane, depending on the number of selected atoms.

1 atom selected:	The molecule is aligned to the axis defined by its centre and the selected atom.
2 atoms selected:	The molecule is aligned to the axis defined by the two selected atoms.
3 atoms selected:	The molecule is aligned to the plane defined by the three selected atoms.

Reset Position
Centre
x,y,z-Rotate ..

General:

These commands supplement the interactive movement by the mouse and a keyboard key.

Reset Position: Resets the molecule to its position when last saved.

Centre: Moves the centre of the molecule to the centre of the working window.

x,y,z-Rotate .. : Rotates the molecule by exactly 90° around the indicated axes in the indicated direction.

Interactive Movement ...

General:

Since the interactive movement of a molecule may not be obvious from the program, it is described schematically in a help window. This window can also be invoked by the "Help"-command of the apple-menu.

Opens the help window shown below:

