MicroWorld

Version 1.2

Reference Manual

Table of contents

Positioning-Menu:

About MicroWorld

MicroWorld is a molecular display program, which calculates three dimensional models (Lines, 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.

- Antialiasing: smooth stick drawing - no more jaggies.
- Depth cueing: model colors become darker (or optionally brighter) with increased 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.
- Colorizing of selected model parts.
- 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.

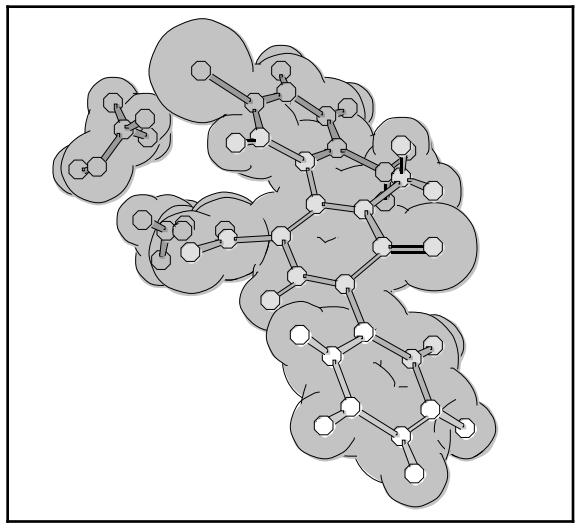
MicroWorld requires system 6.07 or higher, a 68020 processor (or higher) and the presence of color QuickDraw.

Model Types

The basic task of MicroWorld is the conversion of atom coordinates to molecular models. In contrast to e.g. business data, which also can be understood in their numerical form, atom coordinates have to be visualized in order to understand the shape of a molecule.

C1	1.234	-0.981	2.892
C2	2.432	1.434	-7.988
H3	3.123	0.234	9.110
O4	-2.321	1.987	-9.456
...	...	...	...
...	...	...	...

Atoms and their coordinates



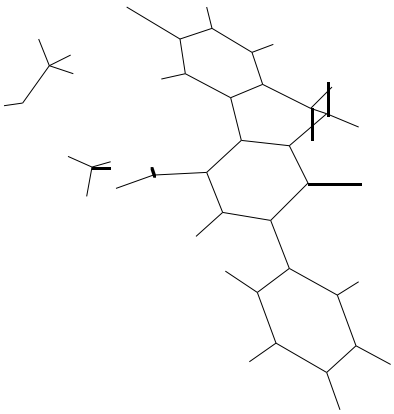
Molecular Model

MicroWorld offers the choice between a wide range of common molecular models - and a few more (see next page). Additionally, different model types can be mixed in one molecule.

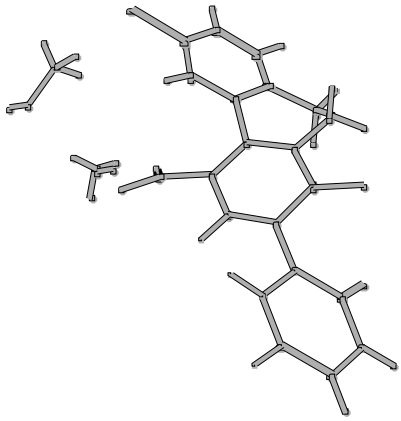
Each of these models may again be represented in three different modes:

- Normal: Standard mode. Full color, shaded, antialiased model representation including all extras. Highest available picture quality.
- Outline: Very fast rendering, producing an unshaded grayscale model representation. Well suited for a quick model preview.
- Printing: Black&white model representation, partially filled with gray areas. Takes advantage of the highest available printer resolution.

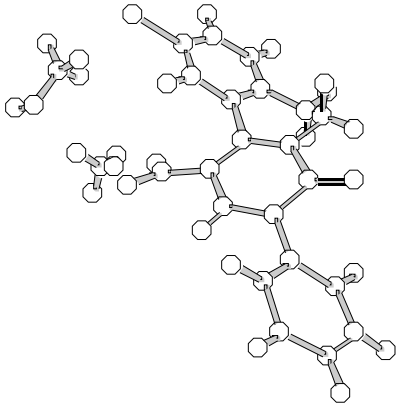
MicroWorld's model types (as Outlines):



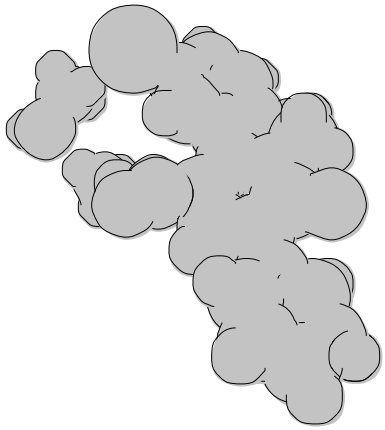
Wire Frame



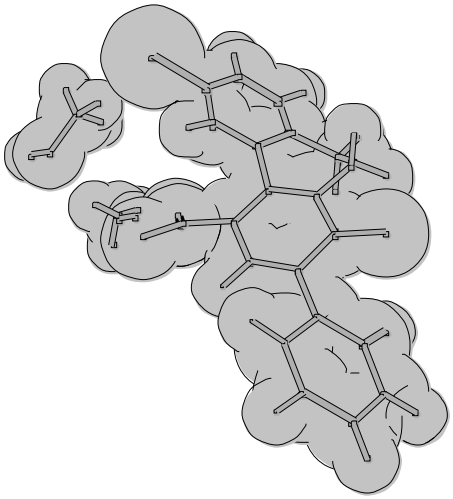
Lines / Dreiding



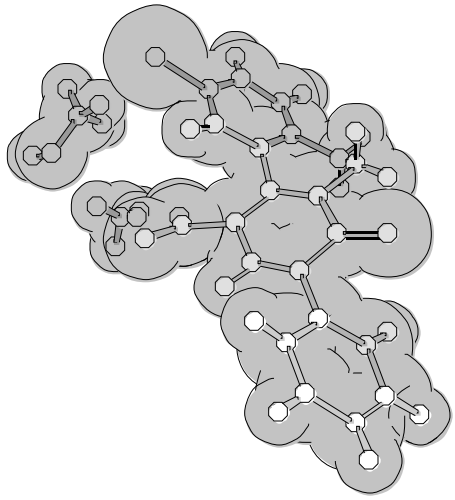
Ball & Stick



Space Fill

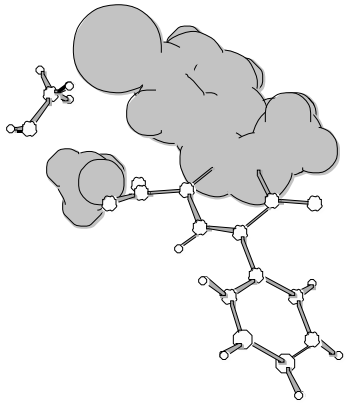


Transparent Space Fill with Sticks

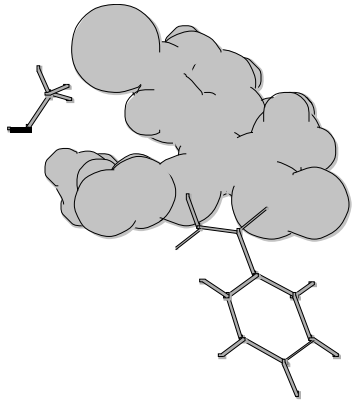


Transparent Space Fill with Ball&Sticks

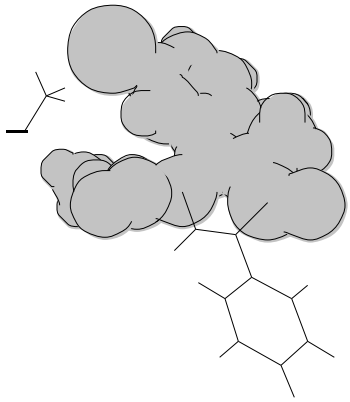
Models can be mixed with each other, even in the same molecule. An example of all possible mixed models containing a Space Fill model (SPF) is shown below.



SPF mixed with Ball&Sticks



SPF mixed with Dreiding



SPF mixed with lines

Interactive movement of the molecule

translation cursor

rotation cursor

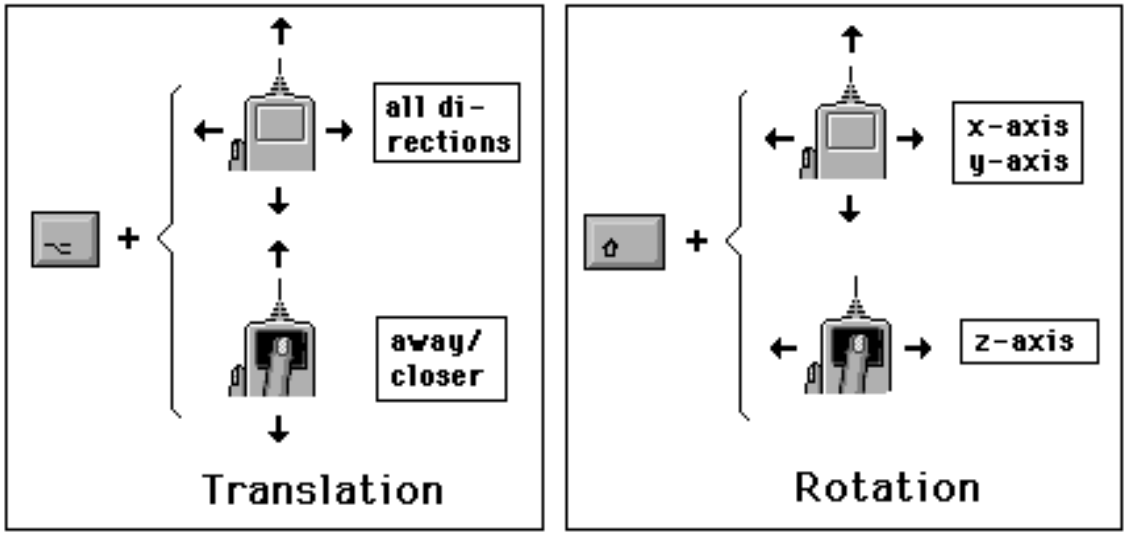
General:

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).

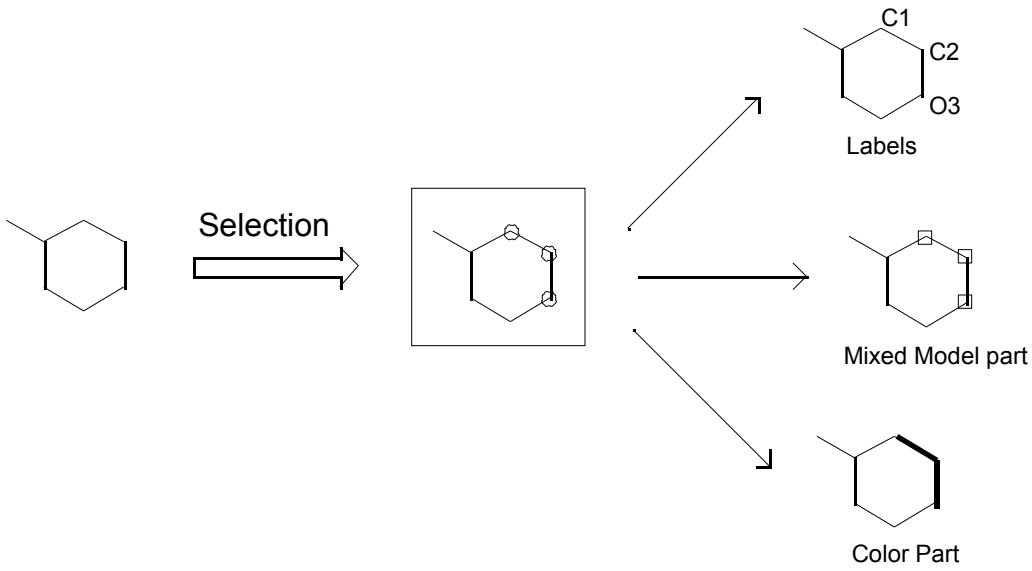
Note: The menu item "Interactive Movement" in the "Positioning" menu provides the picture below as an online help.

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.



Selection of atoms

The selection of atoms is a basic tool of MicroWorld. Selected atoms can be treated in special ways, they can e.g. get labels, appear in a special color or in another model type. All operations influencing selected atoms are available in the "Selection"-Menu.



Selection:

Atoms are selected by clicking them, or by dragging a rectangle over a group of them (drag = move the mouse with pressed mouse button). Selected atoms are marked with small circles.

Clicking an atom while the *command*-key is pressed, will result in the selection of ALL atoms belonging to the same molecule. This is especially useful, when more than one molecule is present in a model.

The "Select All"-command of the "Edit"-menu selects ALL available atoms.

Clear Selection:

The selection of an atom is removed by selecting it again. The "Edit Selection...Clear All"-command of the "Selection"-menu clears the selections of all available atoms.

Clicking an atom while the *ctrl*-key is pressed, will clear the selections of ALL atoms belonging to the same molecule.

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, settings, 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 program settings are overwritten by the file settings, if the option "Allow substitution by MW-file settings" in the color- and/or model-setting is on.
Save...	Saves the actual position and all other relevant data of the displayed molecule, including the settings, as a MW-file. Nevertheless, no copy of the screen picture is saved (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:

In contrast to other common import/export ASCII text formats (e.g. from x-ray measurements, force field calculations, 3D-databases, or similar sources), MicroWorld's import format requires just the essential data for a molecular model construction: the labels and space coordinates. All other data can be extracted from these basic data and are thus not required.

Therefore, almost all external import/export formats can be converted to the MicroWorld import format (see below), by simply removing all the redundant information with a text editor.

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. *It is highly recommended to save the molecule immediately as a MW-file (see "Save").*

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: therefore, the underlying wire frame model appears after a mouse click, which can be moved and edited in the usual way.

The settings stored in a MW-*picture* will always override the ones defined in the model- and color-setting. This is in contrast to a MW-*file*, where the user can choose, whether these settings are overwritten or not ("Allow substitution by MW-file settings"-option).

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, but 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.

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 and color settings are updated.
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).

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 "background 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 1: 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 2: 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 3: The display of a background picture can be switched off temporarily by switching off the "Show background picture"-option of the "Model Settings"-dialog.

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 *wire frame* mode, only a message of the successful installation appears but the background picture will be visible during any subsequent model calculation. In the *color model* mode, the current model is recalculated using the new background.

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

Note: Because of approximations in the generation of space fill models for printers, 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 ...	Prints the current model as black and white graphics. In order to enable the printing of gray areas, "best" or "color/grayscales" should be chosen in your printer setup.
Quit	Ends the program.

Copy Area
Select All

copy cursor 

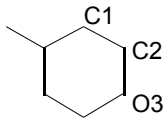
General:

Only the copy commands and the "Select All" command of the "Edit"-menu are currently active. 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 Area:	Copies a selected part of the screen to the clipboard. A copy-cursor (see picture at the top right of the page) appears, with which a rectangle around the area to be copied can be dragged. Its contents are copied to the clipboard, as soon as the mouse button is released.
Select All:	All atoms of the current model are selected. This will immediately switch the model to the wire frame representation.

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



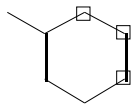
General:

Attaches labels (e.g. Si32, Cu12, C1, ...) to the selected atoms.

Note: The command "Show All Labels" (Model Menu) displays the labels of all atoms, no matter if they are selected or not.

Define/Use	The selected atoms receive a label. In case they already possess a label, this is removed. If no atoms are selected, but some labels are present, their definition is switched on/off by the above command. A checkmark to the left of the menu item indicates that they are switched on.
Clear All	All label definitions are erased and the labels disappear.

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

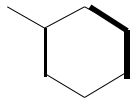


General:

The "Mixed Model"-command defines selected atoms as members of a model within another one, without specifying it's type yet. The latter may be defined in the "Model Settings" (Model-menu).

Define/Use	The selected atoms become defined as mixed model parts. They are marked with a rectangle. In case they already are defined as mixed model parts, their definition is erased. If no atoms are selected, but some mixed model parts are present, their definition is switched on/off by the above command. A checkmark to the left of the menu item indicates that the mixed model parts are switched on.
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.

Part Color ...Define...
Use
Invert
Clear All



General:

Parts of a model can be painted in different colors (color parts), in order to stress out certain parts of the model. Thus, in an enzyme-substrate-complex, the enzyme could be painted e.g. in red, and the substrate e.g. in blue.

Define...	Paints the selected atoms in an arbitrary color, chosen from the appearing color menu: the color of it's item texts corresponds to the available colors (when hilited, the item's background appears in that color). After this definition, such color parts are drawn in their respective color in the wire frame model. Up to 16 different part colors per model can be employed. The "clear selected" command resets the selected atoms to their original element colors.
Use	Toggles between part color and normal color display. When checked, the part colors are in use.
Invert	Resets the color part(s) of the model to the original element colors, and vice versa. Only active, when just one part color is used in the model.
Clear All	All color part definitions are erased.

Edit Selection ... **Invert**
Clear All

General:

Apart from the selection/deselection by the mouse, the selection of all model atoms can be manipulated by the commands below. Additionally, the "Select All"-command from the "Edit"-menu selects all atoms of the current model.

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

Geometrical Info

General:

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

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.

Lines
Dreiding
Ball&Stick
SpaceFill
Transp. SPF+Sticks
Transp. SPF+B&S

General:

The amount of transparecy of the transparent models can be adjusted within the "Model Settings"-dialog (Model-menu). Generally, the appearence of all model types can largely be influenced by the model- and color-setting.

*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.*

Lines:	Calculates a model consisting of antialiased lines in one single color. This line color is assigned in the "Color Settings".
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:	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 menu options are switched on/off by selecting them repeatedly. If they are on, their menu item is checked.

Outlines Only:	Very fast model calculation in unshaded grayscales, but with depth cueing. Useful for quick model previews.
Show All Labels:	The labels of **all** atoms are displayed. During an interacive movement of the molecule they are temporarely switched off.
Full Screen:	The working window is expanded to the whole screen, the menu bar disappears. However, after pressing the mouse button at the very top of the screen, 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 screen pictures.

Model Settings

Preferences icon 

General:

In this dialog window, settings for several parts of the program can be defined. These settings are saved permanently with "SAVE AS DEFAULT", restored with "GET DEFAULT", or used in the current model by clicking the "OK"-button. If necessary, the model will be recalculated when the dialog window is closed.

When a model is saved as MW-file or MW-picture, it's current model- and color settings are included in the file. When a MW-file is opened later on, it's settings will override all current model- and color-settings, if their corresponding option "Allow substitution by MW-file settings" is on. In contrast, a MW-*picture* will always override all settings.

Background:

Background Shadow:
A shadow of the model is cast onto the background (if not black).

Show Background Picture:
The display of a background picture can be switched on/off by this option. If none is 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.

Depth Queing:

Darker With Distance:
The model becomes darker with distance. It is drawn on a black background, if no background picture is present.

Brighter With Distance:
The model becomes brighter with distance (dust effect). It is drawn on a white background, if no background picture is present.

Wire Frame DQ, Outlines DQ, Model DQ, Model-Labels DQ:
Switches the Depth Queing option of each model type and the model labels on and off. If switched off, no change in color brightness with distance occurs.

Display:

Color Legend:
Displays a color legend, which reflects the color assignments of the current model (not visible in the wire frame model). This legend can be dragged to any position in the window.

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

Mixed Model Parts Of...:

Assignment of a model type to the mixed model part (s."Selection"-menu) of a Space Fill or Ball&Sticks model. The Dreiding model can only contain a Lines model, while the Lines model can contain no other model at all.

Allow substitution by MW-file settings:

Allows the substitution of the current model-settings by the ones of an opened MW-file. The current settings are always overwritten by an opened MW-picture.

Color Settings

Preferences icon 

General:

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

When a model is saved as MW-file or MW-picture, it's current model- and color settings are included in the file. When a MW-file is opened later on, it's settings will override all current model- and color-settings, if their corresponding option "Allow substitution by MW-file settings" is on. In contrast, a MW-*picture* will always override all settings.

Element Colors: The desired element symbols are entered into the text fields to the right of the color boxes. Old entries are replaced by clicking their text field and entering the new text, without previously deleting them. 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".

Line Color: Click one of the 16 Element-Color boxes to assign a color to the Lines-model. This color appears in the line color box.

Get Default: Resets all color assignments to the values saved with the "Save As Default"-command.

Save As Default: Saves the current color assignments in the preferences file. They can be recalled with the "Get Default"-command.

Allow substitution by MW-file settings:
Allows the substitution of the current color-settings by the ones of an opened MW-file

OK: The color assignments will be used in the current model.

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: