MicroWorld

a molecular display & analysis program

Reference Manual

Version 2.0

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About MicroWorld

MicroWorld is a molecular display and analysis program. It calculates three dimensional models (Lines, Dreiding, Ball&Stick, Space Fill) from 3D atom coordinates, e.g. from x-ray data, 3D-databases, publications or other chemistry software. It features powerful functions which are, so far, quite rare with other programs of this kind.

- Fast antialiasing: smooth stick drawing.
- Depth cueing: model colors become darker 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.
- Coloring of selected model parts.
- Fast search functions: element, label, group (exact or substructure, interactive or non-interactive), protein and DNA/RNA backbone, find in radius.
- Alignment of the model to a point, a bond, or a plane.
- Display of a color legend for element colors.
- Mathematical coprocessor not necessarily needed.

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

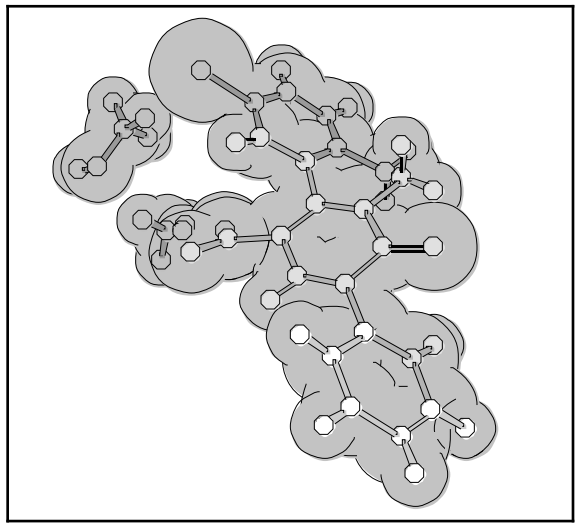
If you are a user of the shareware utility "Greg's Buttons", you have to switch off all of its colorizing options (finder windows, menus, dialog boxes & alerts) before running MicroWorld, because of a compatibility problem.

Model Types

The basic task of MicroWorld is the conversion of atom coordinates to molecular models.

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 coordinates

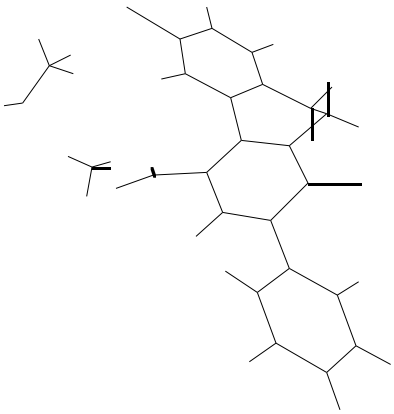


Molecular Model

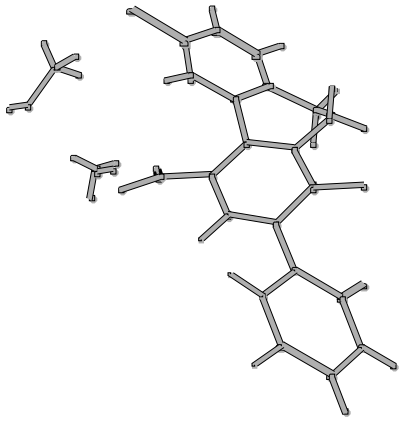
MicroWorld offers the choice between a wide range of molecular models (see next page). Additionally, different model types can be mixed within one molecule.

A very fast rendering in unshaded grayscales is provided for quick model previews (outline mode). This is especially useful on slower machines.

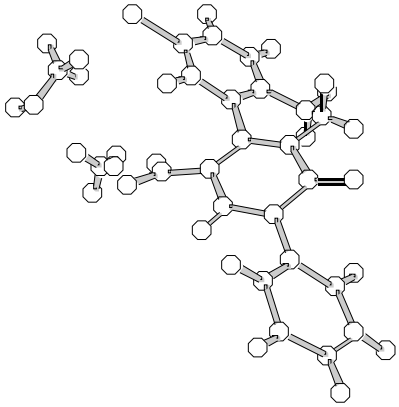
MicroWorld's model types (as Outlines):



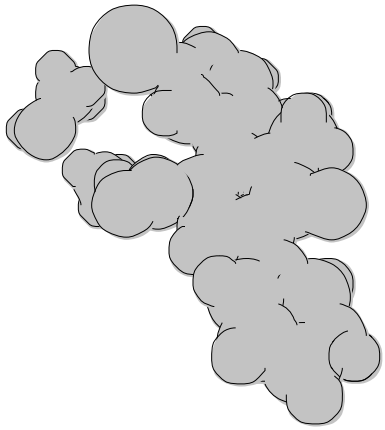
Wire Frame



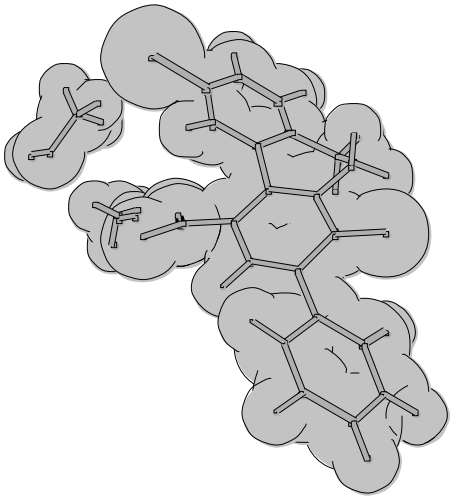
Lines / Dreiding



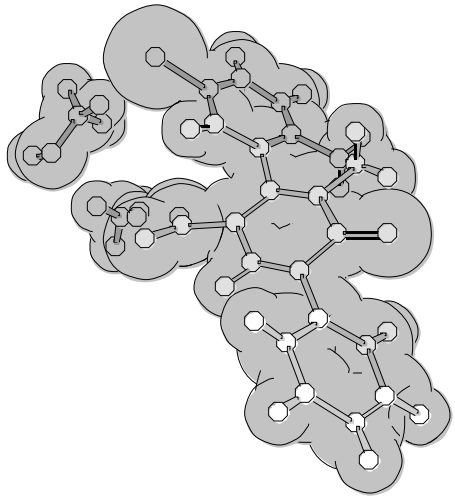
Ball&Stick



Space Fill

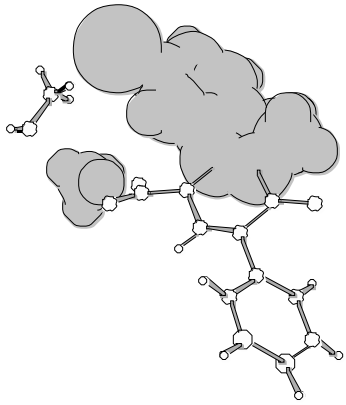


Transparent Space Fill with Sticks

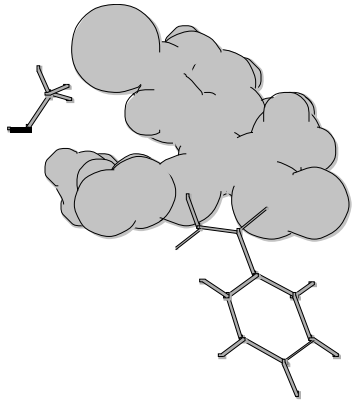


Transparent Space Fill with Ball&Sticks

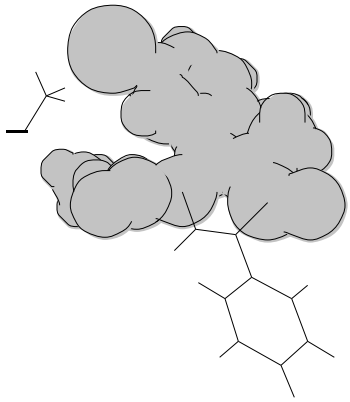
Models can be mixed with each other, even within the same molecule. An example of all possible mixed models containing a Space Fill model (SPF) is shown below.



SPF mixed with Ball&Sticks



SPF mixed with Dreiding



SPF mixed with lines

Interactive animation of the molecule

translation cursor

rotation cursor

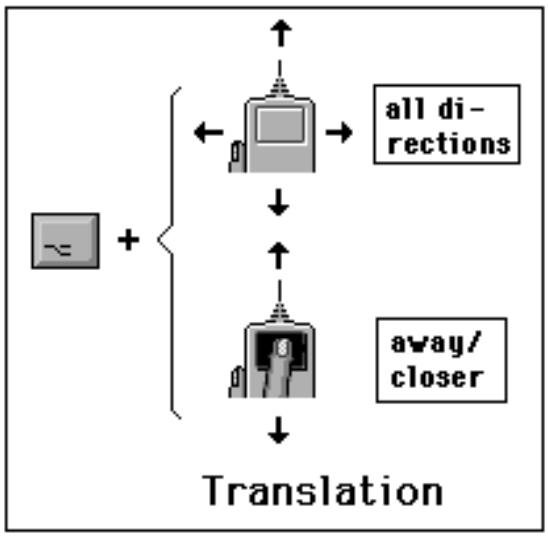
General:

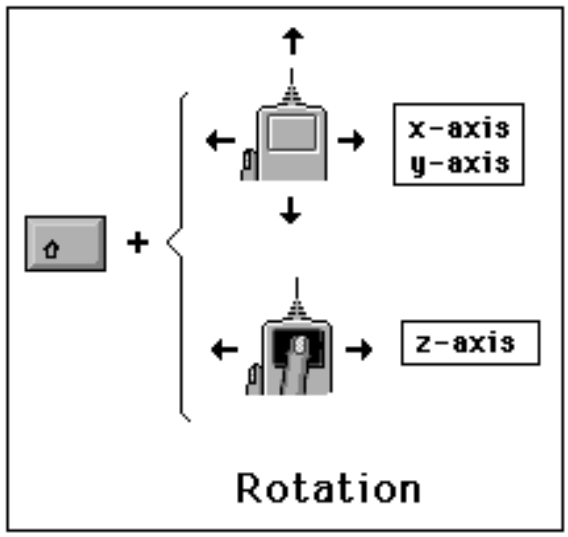
A molecule is rotated and shifted by the simultaneous use of the mouse, a keyboard key and sometimes the mouse button, as shown below.

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

Note: The menu item "Interactive Animation" in the "Positioning" menu, as well as the "Help..." item in the Apple-menu, provides the picture below as an on-line help.

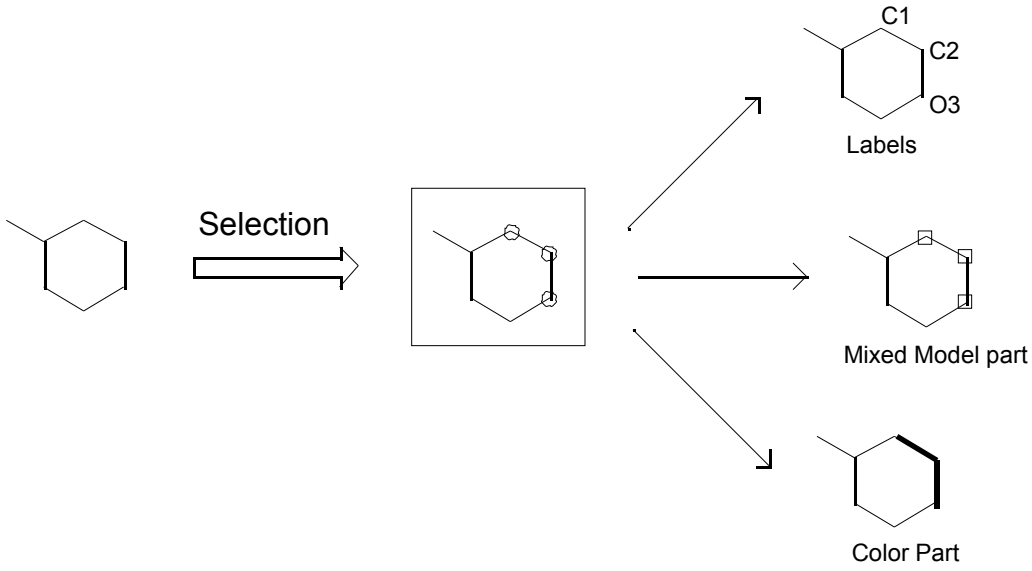
Rotation:	When pressing and holding the **shift**-key, the rotation cursor appears (see picture at top of page). Any subsequent mouse movement with the shift-key still depressed will rotate the molecule around its x- and y-axis. With the mouse button pressed, a horizontal mouse movement will cause a rotation around the z-axis.
Translation:	When pressing and holding the **option**-key, the translation cursor appears (see picture at top of page). Any subsequent mouse movement with the option-key still depressed will shift (translate) the molecule in any direction on screen. With the mouse button pressed, 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. be assigned 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.

For the selection of all atoms belonging to the same molecule, simply click one of it's atoms with the *command*-key pressed. 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 cleared by re-selecting it. The "Edit Selection... Clear All"-command of the "Selection"-menu clears the selections of all available atoms.

Clicking an atom with the *ctrl*-key pressed clears 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 pixel copy of the screen picture.

The settings stored in MW-files only overwrite the current color- and model-settings, if the option "Protect settings" of the latter is off.

The "Demo-MW-files"- folder on the program disk contains examples of MW-files.

Open ...	Opens a model in wire frame representation in exactly the state it was last saved.
Save...	Saves all relevant data of the displayed molecule, including all settings.
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 features an import mechanism, which allows the import of 3D atom coordinates from a wide range of applications after a minimum of editing. These data need to be in ASCII (text) format and are in most cases easily converted to MicroWorld's import format by cutting all redundant data above and below their coordinate part in a text editor. There is a limit of 500 atoms per model and of 8 bonds per atom.

In organometallic complexes like e.g. ferrocene, the connection between the η^5 or η^6 ligand and its metal centre is represented by a single bond originating from the centre of the ligand ring to the metal atom.

Please note that most external coordinate formats cannot be imported without some prior editing.

If all coordinate values are smaller than 2, or if some are larger than 250, then fractional data are assumed and a dialog window for the input of the required unit cell data appears. Otherwise, the import mechanism will, based on distance and geometry criteria, try to estimate atom connections and a correct coordinate scaling (in Angstrom units).

Note 1: If a scanner is used for input, please make sure that it's software will properly distinguish the letter "O" from the number zero "0", the letter "l" from the number "1" and will not read a 0.123.. as 0-123 etc.

Note 2: Special formats, like alpha carbon chain models, represent their atoms in 'unnatural' configurations and will therefore cause import errors .

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.

(continued on next page)

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. If the import is successful, the molecule is successively represented as wire frame model. *It is highly recommended to save the molecule 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 picture file (PICT-format), which is accessible by virtually every graphics application on the Mac. In addition to these standard picture data, and invisible to other programs, a MW-picture 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 and can be moved and edited in the usual manner.

The settings stored in a MW-*picture* 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 ("Protect 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). 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. 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.

The "Backgrounds"-folder contains examples of background pictures.

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: 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 or outline mode, only a message of the successful installation appears, but the background picture will be visible during any subsequent full color model calculation.

Page Setup ...
Print ...
Quit

General:

The best and, at the same time, least expensive method for the reproduction of color-computer graphics is to photograph a picture from the screen. 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 monitor 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").

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 

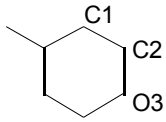
General:

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



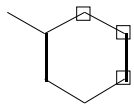
General:

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. Uncheck this item to temporarely deactivate all label definitions. Check it again to reactivate these definitions.
Clear All	All label definitions are erased and the labels disappear.

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

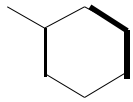


General:

The "Mixed Model"-command defines selected atoms as members of a model within another one: e.g. portions of a Space Fill model may be displayed as Dreiding model. The actual type of such a sub-model is specified by the pop-up menus in the "Model Settings" dialog (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, all mixed model part definitions currently present are activated/deactivated by the above command. A checked menu item indicates activated definitions.
Invert	All atoms **not** defined as mixed model part now become defined as such and vice versa.
Clear All	All mixed model part definitions are erased.

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

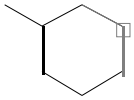


General:

Parts of a model can be painted in different colors (color parts), in order to highlight 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 and bonds between them in the arbitrary color chosen from the appearing choice of 12 colors. Single colored atoms (no colored bonds) are only visible in the Ball&Stick and Space Fill models. The "clear selected" command resets the selected atoms to their original element colors.
Use	If you uncheck this item, the part color definitions are temporarily ignored. Check it again to reactivate these definitions.
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.

Hide ... **Define**
Use
Invert
Clear All



General:

Parts of a model can be hidden by this command. In the wire frame model they appear as dotted lines with faint yellow atom centres. They are invisible in all other models.

Define	All selected atoms become hidden. Already hidden ones become unhidden when selected.
Use	Uncheck this item to temporarely deactivate all hidden atom definitions. Check it again to reactivate them.
Invert	Defines all unhidden atoms as hidden and vice versa.
Clear All	All hidden atom definitions are erased.

Invert Selection
Clear Selection

General:

In contrast to the manipulation of single atoms or groups of them by the mouse, the commands below manipulate ALL model atoms.

Note: *The "Select All"-command from the "Edit"-menu selects all atoms of the current model.*

Invert:	All unselected atoms become selected and vice versa.
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.

Click anywhere on the screen or animate the model to continue.

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. Each angle is assigned to the corresponding centre.

Find Analogous.. **Same Group**
Similar Group

General:

The Find Analogous commands are the interactive versions of the "Find Group" command in the Search-menu.

Same Group:	Selects all atoms having exactly the same substituents as the currently selected one (exact search).
Similar Group:	Selects all atoms having exactly the same substituents as the currently selected one, plus any others (substructure search).

Select in Range.. **From Selected to Front**
From Selected to Back
From Selected to Radius...
Of Same Molecule

General:

These commands are valuable tools for the selection of specific parts of a model. Note, that left, right, top and bottom parts of a model are easily selected by dragging the selection rectangle over the desired area.

From Selected to Front:	Selects all atoms between the currently selected one and the viewer.
From Selected to Back:	Selects all atoms between the currently selected one and the most distant one from the viewer.
From Selected to Radius..:	Selects all atoms within a specified radius from the currently selected one. Enter the desired radius in the appearing dialog box.
Of Same Molecule:	Selects all other atoms of the same molecule. Note that the same effect is achieved by selecting an atom with the *command*-key pressed. The selection of an atom with the *ctrl*-key pressed deselects all atoms of the same molecule.

Make Bond
Break Bond

General:

The commands below provide the tools for editing connections between atoms.

Make Bond:	Creates a bond between the two selected atoms.
Break Bond:	Removes the bond between the two selected atoms.

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

General:

The appearence of all model types can largely be influenced by the model- and color-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.*

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. The amount of transparency is specified in the "Model Settings".
Transp. SPF+B&S:	Calculates a Space Fill model and then overlays a transparent Ball&Stick model. The amount of transparency is specified in the "Model Settings".

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, not antialiased 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. The settings are applied to the current model by clicking the "OK"-button. If necessary, the model will be recalculated when the dialog window is closed. The current settings may be saved with "MAKE DEFAULT", which makes them show up as default settings after every program start. The last saved settings default can be activated with "GET DEFAULT".

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

Background:

Background Shadow:
A shadow of the model is cast onto a background picture (if present).

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

Depth Queing:

Depth queing is a form of a graphic representation in which model parts become gradually darker with increasing distance to the viewer, resulting in an enhanced impression of spatial depth.

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 occurs with distance.

Display:

Color Legend:
Displays a color legend which reflects the color assignments of the current model (not visible in the wire frame and Lines models). Part color assignments are not reflected. 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.

Protect Settings:

Protects the current model-settings from overwriting by a MW-file. Note, that the current settings are always overwritten by a MW-picture.

Get Default: Resets all assignments to the values saved with the "Make Default"-command.

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

Color Settings

Preferences icon 

General:

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

The settings are applied to the current model by clicking the "OK"-button. If necessary, the model will be recalculated when the dialog window is closed. The current settings may be saved with "MAKE DEFAULT", which makes them show up as default settings after every program start. The last saved settings default can be activated with "GET DEFAULT".

When a model is saved as MW-file or MW-picture, it's current model- and color settings are included in the file. When such a file is opened later on, it's settings will override all current model- and color-settings, if their corresponding "Protect Settings" options are off. In contrast, a MW-*picture* always overrides all settings.

Element Colors: The desired element symbols are entered into the text fields to the right of the color boxes. 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 12 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 "Make Default"-command.

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

Protect Settings:
Protects the current color-settings from overwriting by a MW-file. Note, that the color settings are always overwritten by a MW-picture.

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 animation.

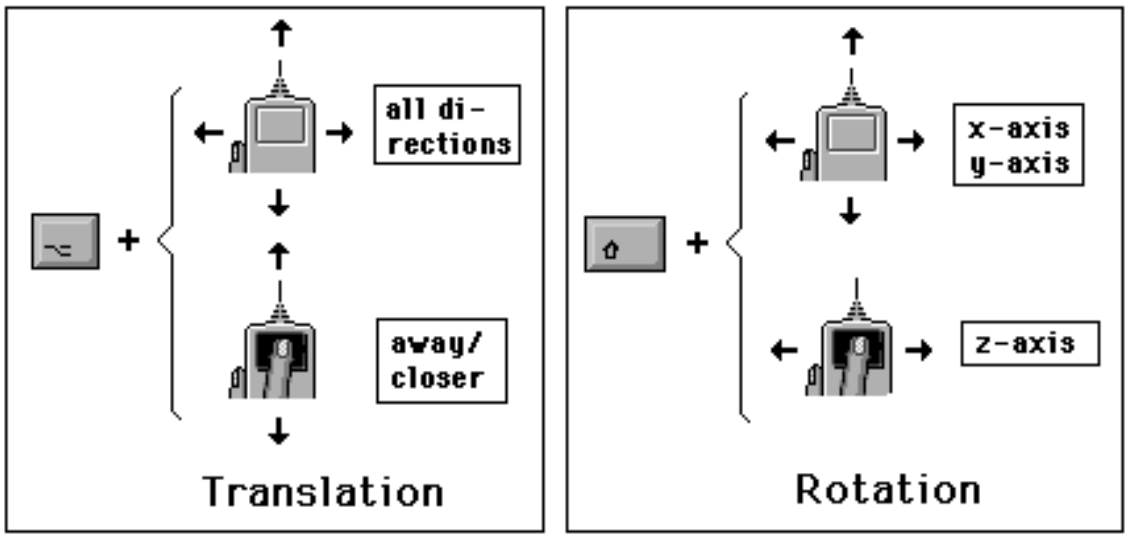
Reset Position:	Resets the molecule to its position when last saved.
Centre:	Moves the centre of the molecule to the centre of the working window.
x,y,z-Rotate .. :	Rotates the molecule by exactly 90° around the indicated axes in the indicated direction.

Interactive Animation ...

General:

This is an informational help window. It can also be invoked by the "Help"-command of the apple-menu.

Opens the help window shown below:



Element
Label

General:

These commands allow the selection of atoms according to specific criteria.

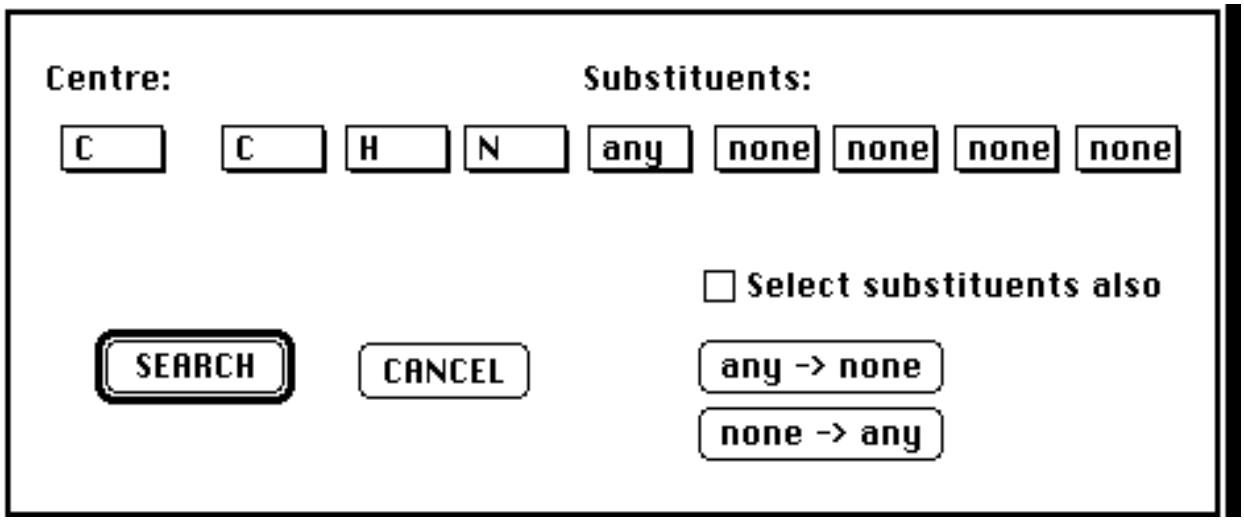
Element:	All occurrences of the element specified in the appearing elements-submenu become selected in the model.
Label:	Specify a label (e.g. 'C132') in the appearing dialog box. If 'partial match' is off, then the atom with exactly the specified label becomes selected. If 'partial match' is on, then all atoms containing the specified label as part of their own label become selected; e.g. if 'C2' is specified, then 'C2', 'C21', C22',... could become selected; if '23' is specified, 'C123', 'N23', 'O223',... could become selected.

Group...

The group command allows the search for specific groups. A group is defined as a central atom connected to a number of substituents. Most organic functional groups like esters, aldehydes, nitriles, etc. can be defined as such a group. But please note that a functional group definition is only unambiguous if the model contains hydrogens.

The Group command invokes the dialog window below. Its pop-up menu's contain exactly the elements present in the current model. Additionally, the options **any** and **none** are available for all pop-up's (except **none**, which is not available for the central atom).

When opened for the first time after loading the current model, the menus of the group-dialog are all set to **any**. If exactly one atom is selected in the current model before opening the group-dialog, then the menus reflect the configuration around this specific centre.



any:	This attribute allows any kind of central atom or substituent, including no substituent at all. It is used for substructure searches.
none:	This attribute excludes any substituent.
any->none:	Changes all **any** attributes to **none** attributes. Useful for converting a substructure search to an exact search.
none->any:	Changes all **none** attributes to **any** attributes. Useful for converting an exact search to a substructure search.
SEARCH:	Looks for the specified groups in the current model. If found, the corresponding central atom is selected.
Select substituents also:	Selects also the substituents, if a group is found.

(continued on next page)

A search may contain **any** and **none** attributes at the same time, thus defining a restricted substructure search.

Group-search examples:

C - C,C,C,C, none, none.... Selects all quarternary carbons.

C - O,O,C,H, none, none.. Selects all primary acetals (only if model contains H's).

C - O,O,C,C none, none.. Selects all secondary acetals.

C - O,O,C,any, none, none.. Selects all acetals, esters and acids.

any - N, N, N, N, any, any... Selects all centres connected to 4 nitrogens and possibly some more substituents.

Mg - any, any, none,none,... Selects all Mg atoms (ions) connected to a maximum of 2 substituents.

P - O,O,O,O, none,none,... Selects all phosphate groups.

All these searches occur very fast. In quite large molecules, the search could take up to 1 second (measured on a mid-range Mac).

Protein Backbone
DNA/RNA Backbone
Unconn. Atoms ...

General:

As with the group search, also this search is also quite fast: even the two DNA backbones of a double helix, together consisting of about 500 atoms, become selected in less than 1 second on a mid-range Mac.

Protein Backbone:	All atoms forming the protein (or peptide) backbone become selected.
DNA/RNA Backbone:	All atoms forming the DNA/RNA backbone become selected. For aesthetic reasons, the oxygens of the phosphate group are also selected.
Unconn. Atoms:	Selects all atoms which are not connected to others. This is a tool for detecting water (if no H's present) or ions 'floating' in and around a crystal structure.