Chapter 4
Working with Groups

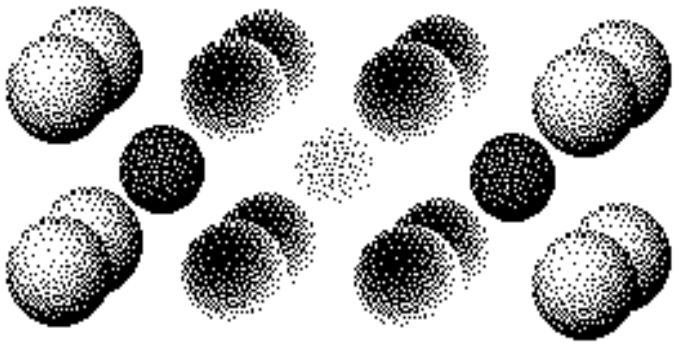
Introduction

MacAtoms version 3 allows you to arrange atoms into groups that can be manipulated as entities. You can use this capability in a number of ways. For example, you can select a number of atoms and cut them from the picture, thus letting you look inside a molecule. You can make a copy of a selection and paste it into another window where you can take a closer look at it. You can move the selection to one side, perhaps rotating it in the process, again with the intent of looking inside a molecule. You can take a selection of atoms and combine them into a single group. When this is done, you can select the entire group by clicking on any of its component atoms. Groups can also contain other groups. You might use this to build up a molecule out of simple components, each of which is itself a group of atoms and/or other groups. This chapter discusses how to work with selections to accomplish some of these things.

There are two ways to establish a group of atoms. You can arrange atoms into predefined groups using the data file, or you can select one or more atoms and form them into a group using the Group command from the Action menu. We will concentrate on interactively defined groups in this chapter, and discuss data file groups in the next chapter. Once a group has been established, it works the same no matter how it was created. In particular, groups defined in a data file can be manipulated by the techniques described in this chapter.

Making a selection

To select atoms interactively, you must use either the Select One or Select Many tool from the Tools menu. The action of the Select One tool depends on where the mouse is clicked. If the mouse is clicked when the cursor is over an atom, that atom is selected. If there are several atoms under the cursor, the one closest to the viewer is selected. You can tell which atoms are selected because they appear with their contrast reversed, as shown in the following example where the nine of the atoms near the center have been selected.



If you have selected one atom and then click on another, the first atom will be deselected and the second will be selected. However you can use the standard shift-clicking technique to build up a selection of several atoms. For example, if you have selected a single atom and hold down the shift key while you click on another atom, then both atoms will be selected. If you shift-click on the atom a second time, it will be deselected, leaving only the first atom selected. You can use shift-clicking to

build ever larger selections by adding one atom at a time.

Normally, only a single atom will be selected when you click on it, but if your selection happens to belong to a group, then the entire group will be selected and highlighted. Shift clicking can also be used to combine groups.

So far we have assumed that the Select One tool has been clicked over an atom. If instead it is clicked over an empty area, it acts like the Select Many tool. To use that tool in turn, press the mouse button, drag the mouse to another place, and release the button. As you drag the mouse, an outline of a rectangle is displayed so you can see what you are selecting. When the mouse is released, all atoms under the rectangle will be selected, regardless of depth. If one of the selected atoms happens to belong to a group, the entire group is selected, even if some of its atoms fall outside the selection rectangle. The Select Many tool can also be used with the shift-clicking technique. For example, you might select a group of atoms using the Select Many tool, then use the Select One tool to add or remove individual atoms from the selection.

Up to now, we have said that the individual atoms in a group cannot be selected, since selecting one atom in a group will cause the entire group to be selected. One way out of this is to ungroup the atoms as discussed below, but that can be inconvenient. Another way is to use an option-selection technique. To use this technique, place the cursor over an atom, then hold down the option key and press the mouse button. In this case only the atom itself will be selected even if it is in a group; the other atoms in the group will not be affected. Note that selecting the atom does not extract the atom from the group but just selects the atom for further study. You can combine shift-selection with option-selection. Thus, by holding down both the option and shift keys while making a selection, you can select a single atom from a group and combine it with a previous selection. The option-selection technique works with both the Select One and Select Many tools.

What to do with a selection

Once you are satisfied with the selection, there are several things you can do with it: make it into a group, ungroup it, move it, and cut and paste it. We will discuss these in turn. Note that as a general rule, if you have selected nothing, the program will assume that you want to work with all the atoms.

Forming a group

Once a selection has been made with the mouse, you can use the Group menu command to gather the selected atoms into a group. This group may itself contain other groups and so on. Groups do not lose their identity when they are put in another group, so when you go to ungroup later, they will reappear.

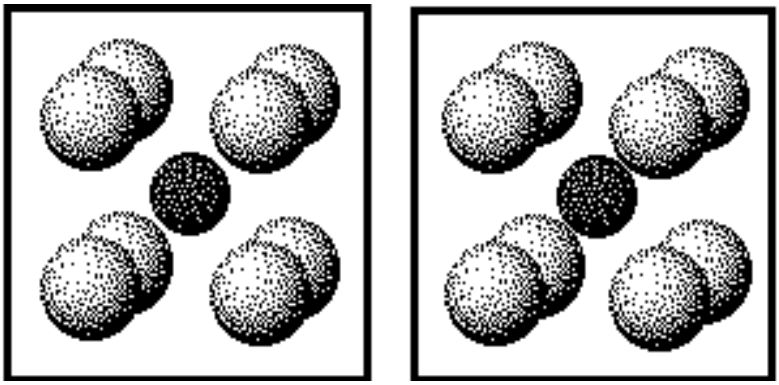
Ungrouping

As indicated above, atoms can be grouped together either interactively or by way of the data file. Once the atoms are in a group, then can only (conveniently) be manipulated as a group. There may be times when it becomes necessary to break up a group so as deal with the component parts. This can be done by using the Ungroup command from the Action menu. Note that the ungroup command does not break up the subgroups; to do that, you would have to enter the ungroup command again one or more times.

Moving a selection

You can move the selection by selecting the Angle, Turn, or Move tool from the Tools menu, then dragging the mouse to prescribe how much change is to be made in the corresponding viewing parameter. Only the atoms that are selected will be moved; the others will not be affected.

You can use this technique to make stereo pairs. To do this, make a copy of the atoms, move it to one side, and change its orientation slightly. The following example shows a stereo pair generated using this technique.



MacAtoms does not throw away the transformation matrix after it has been applied to the atom coordinates. Rather it remembers each individual group's transformation parameters. This feature can be used in several interesting ways. One way would be to read in a set of atoms that have been arranged into groups, then interactively move one group of atoms to the side. That done, you would read in a second set of atom coordinates arranged into the same groups. You would see a display in which the one group has been moved to the side by the same amount as in the first set. By repeating the process, you could make a movie in which the one group is always moved to the side by the same amount.

Another interesting way to use grouping is to make a data file with several *move commands, each of which moves a particular group by a different amount. This would give you a movie in which, for example, the atoms in that group gradually move to the side so as to expose the interior of a structure. Read the next chapter to learn more about how groups are specified in the data file.

It would be impractical and not very useful for MacAtoms to assign a different transformation matrix to each atom, so when the program writes data to a save file, only group transformation matrices are written. At times, a group's transformation matrix will be ill-defined, for example when not all atoms in the group have been moved the same. Therefore, don't be surprised if the data in the file doesn't come out the way you expect.

Cutting and pasting

Besides moving the selection, you can also copy the selection to the clipboard or cut it from the display. You might use this to make a duplicate of a molecule, to copy atoms to another window, or to remove from the picture some atoms that are obscuring your view. Note that copying and cutting are only useful for moving data around withing MacAtoms. The data that is on the clipboard is lost as soon as you leave the program.

Cutting and pasting can produce unexpected effects depending on what groups you have established in the source and target windows, what colors and atom radii have been established there, etc. MacAtoms will behave deterministically, but it may not always do what you expect. For example, if you cut atoms from a particular group in one window and paste them into another window, the atoms will find their way into the corresponding group in the new window (if it exists; otherwise the group will be created.) That can be convenient if the atoms were cut from the target original some time in the past in order to work with them in another window, and now you are returning them to their original window. Presumably you expect the atoms to find their way back to their original groups. You would especially want this behavior if you had cut some atoms by accident and were trying to paste them back to undo the mistake. However a consequence of this is that pasting atoms into a window can sometimes cause atoms to find their ways into unexpected groups.

As another example, if the atoms of a particular type are smaller in the source window than in the target window, then pasting into the target window will cause the atoms to grow in size. That will seem to be sensible if you think that the size of a particular type of atom should be kept consistent within any one window, but it will seem wrong if you expect the atom sizes to stay unchanged when they move from window to window.

The situation can become very complex if the source and target groups have undergone different transformations. MacAtoms tries to remember each group's transformation so that it can be reported in the saved data file. But this cannot always be done economically, especially if different atoms in a group have been transformed in different ways. The consequence of this is that there will be occasions when MacAtoms cannot restore an atom to its original position after the reset command is given. This kind of behavior is especially likely if you use the option-selection technique discussed above, or move atoms from window to window.

Note that most of the problems described above do not occur very often in practice, and then they can be handled with careful planning. For example you can assign type and group numbers so that they don't accidentally get confused with values used in another window, or you can simply paste the atoms into a window that's known to be compatible with the source window -- for example, an empty window. Likewise, you can avoid using the option-selection technique.