MacChemtab

Version 2.0
Users Manual

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Table of Contents

__Introduction__

System Requirements

MacChemtab 2.0 will (hopefully) run on any Apple Macintosh computer. You must have System 6.0.x or System 7.0.x to run MacChemtab. MacChemtab will work with black & white, monochrome, or color monitors, however if you want to use color in the graphing module you must be running System 7.

MacChemtab uses very little system memory, <128K to be exact. The program should be run in a 256K memory partition because of some minor memory problems (see the README file). The program takes up slightly less than 100K of disk space, so it will fit on a System 6.0.5 System Disk and run on a Macintosh SE with 1MB of memory. This makes MacChemtab an ideal program for the classroom environment.

General Overview

MacChemtab is a database of the periodic table of the elements. With MacChemtab, one can easily explore the relationships that exist between the elements in the periodic table. By design, the database is easy to use. It is, therefore, ideal for the educational environment. MacChemtab was designed for introductory high-school level chemistry courses as an add-on to the, "Introduction to the Periodic Table," section. It works well in the classroom environment to provide students with:

• An introduction to databases on a computer. It shows students how useful a computer is for storage and retrieval of complex information.

• An introduction to the periodic table by providing students with an easy, efficient way to retrieve sets of elements and display them in a list, a graph, or in the periodic table.

There are two general steps involved in using the database:

1: Define a set of elements by creating search parameters.

2: Display the elements using one of the predefined forms.

Section 3 of this manual describes how you can create, edit, and delete search parameters to define a group of elements. Section 4 describes how you can view this information, and in some cases, manipulate it.

Viewing a Single Element

MacChemtab functions are accessed through the Macintosh Menu Bar. One of the most basic functions of any database is to display information. MacChemtab allows you to view all the information the database has to offer on each element. To do this, select *Single Element* from the *View* menu and you will see a dialog box similar to figure 1.
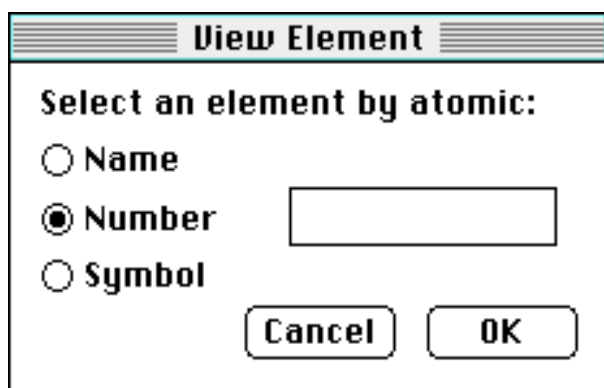

Figure 1

On the left there are three radio buttons. They are labeled Name, Number and Symbol. If you know the atomic name, atomic number or atomic symbol of the element you wish to view, make sure the corresponding name, number or symbol radio box is checked. Next, type in a name, number, or symbol and it will appear in the text box on the right. Click on the OK button to display the element, or cancel to cancel this operation and try something else.

You may enter the atomic name in any fashion, upper or lowercase. The database converts the information you supply into a generic fashion to search for an element. You may also type in part of the element's name. If, for example, you want to view the element Technetium, you may enter Technetium, TeChNeTiUm, TECH, tech, etc. If you enter a name that applies to more than one element, you will receive an error message that tells you the name is ambiguous. If you see this error message, be more precise when typing in the name of the element.

When entering the atomic number, you must type in the exact number of the element you are looking for. You cannot substitute words for numbers (i.e. forty-three instead of 43).

When entering the atomic symbol, you must type in the symbol exactly as it is defined in the periodic table. As a rule, symbols with one character such as the symbol for Oxygen, 'O,' are uppercase. If the symbol contains two or three letters, for example Unnilhexium or 'Unh,' the first letter will be in uppercase and the rest in lowercase. If you enter valid information into the fields and click the OK button, you will see a small window with all the element's information in it. That window looks similar to figure 2, which is an information window for Technetium.

technetium

Atomic Name : technetium
Atomic Symbol : Tc
Atomic Number : 43
Atomic Mass : 98.000 a.m.u.

Melting Temp : 2172 °C (3942 °F, 2445 °K)
Boiling Temp : 4877 °C (8811 °F, 5150 °K)

Specific Heat : 0.580 Calories/gram-°C
Density : 11.50 gram/cm cubed
Atomic Radius : 1.47 Angstroms
Electronegativity : 1.9
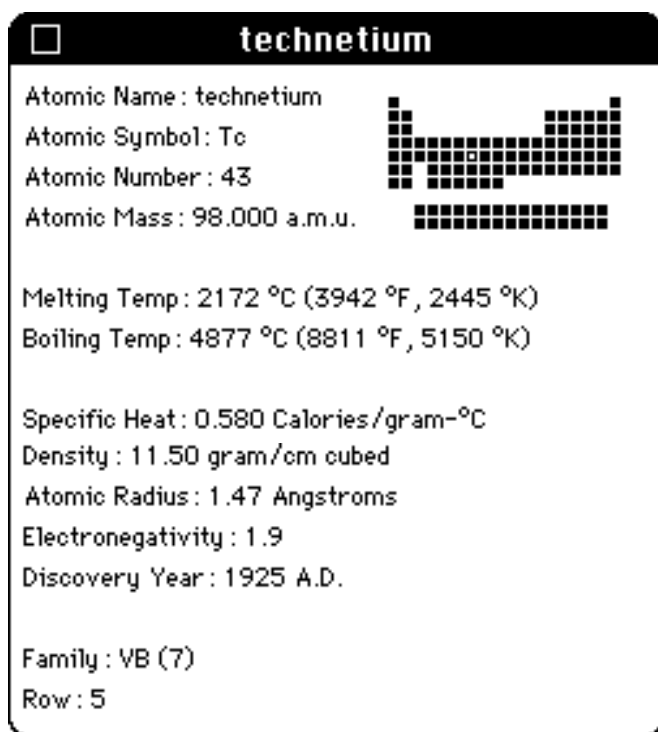Discovery Year : 1925 A.D.

Family : VB (7)
Row : 5

Figure 2

Search Parameters

What is a Search Parameter?

A search parameter allows you to select a group of elements that meet certain criteria. With a single search parameter, for example, you can find all the elements that have a melting temperature greater than 2000ºC. If you create a parameter such as this one, you can filter out elements that you do not wish to study. Let's create this search parameter so you can see what it will do for you. To create a parameter, select *New Search Parameter* from the *Select* menu. A dialog box will appear which is similar to figure 3.
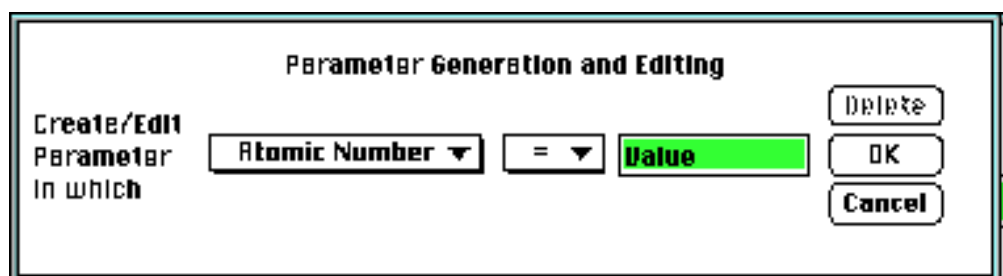

Figure 3

The *Atomic Number* and = boxes are actually pop-up menus. If you move the pointer to one of these boxes and hold down the mouse button, you can see all the searches available to you. As you create the search parameter, read the text in the window from left to right. Currently the window can be read as, "Create Parameter in which *Atomic Number* is = *Value*." We want to change the window to say, "*Melting Temperature* is > *2000*." First, use the left-most pop-up menu and select *Melting Temperature*. Change the = in the middle pop-up menu to >. Now, type in the value 2000.

You will notice that there are three buttons. At this point, you can click on OK to create the search parameter. Click on cancel to forget creating the search parameter so you do not change any information. The Delete button is grayed out because you have not yet created this search parameter, so you cannot delete it yet. After you click on the OK button, the database will find all the elements that meet the search parameter. After doing this, the Select menu will be updated and a new menu choice will be added. The updated menu will look like figure 4.
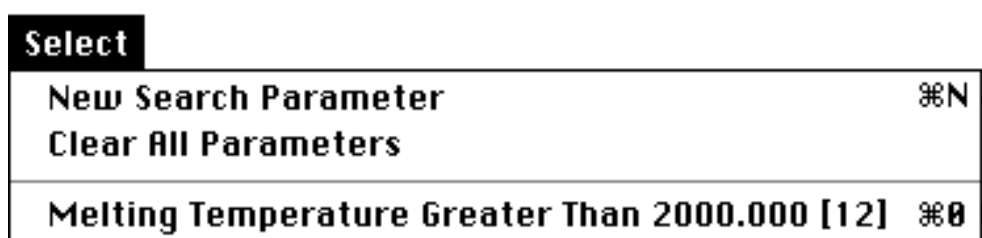

Figure 4

The menu item shows you the search parameter, the number of elements that meet the search parameter, and a hot-key definition for the parameter. The number of elements that meet the search parameter is displayed in brackets ([12]). If you select the search parameter from the Select menu (or in this case hit CMD-Zero), you will see a window similar to figure 3, however it will be updated to show the parameter. You can then edit the parameter and click on OK, or click on Delete to remove the parameter from the list.

You may create up to ten search parameters. After you create each consecutive search parameter, the *Select* menu is updated with the new entry, however the number in brackets represents the number of elements that meet all the previous parameters, including the one you just created.

What is a Close-to Value?

One of the selections under the = pop-up menu in figure 3 is ~. This represents a close-to parameter. By creating a close-to parameter, you find all the elements that are within a certain range from the value you specify. For example, if you specify 10 as the value and the close-to range is 3, you will find 7 through 13. Creating a

close-to value has the same effect as creating two different search parameters, one greater than the smallest value you are looking for and one less than the largest value.

How do I Change Close-to Values?

There are two points in the program from where you can change the close-to values. If you create a search parameter of the close-to type, you will see a number appear below the value you type in. If you click on that number, you can change that close-to value. (That number is the close-to value for the characteristic in the left-most pop-up menu.) If you click on the number, you will see a dialog box similar to the one in figure 5. It is called the mini close value editor.
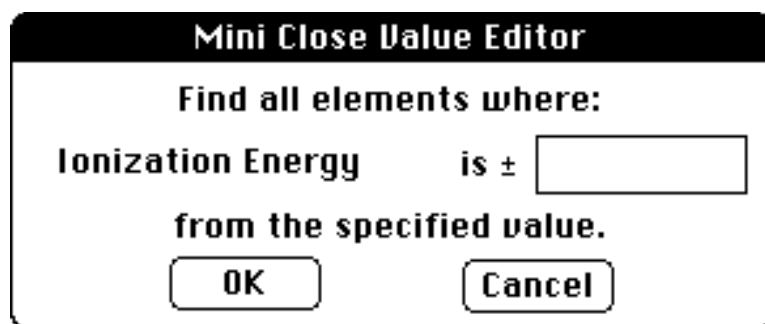

Figure 5

You can type in a new close-to value and click the OK button to change it, or click on the cancel button to leave the value alone. You cannot save the close-to values to the disk with the mini close value editor. To do this, you have to use the close value editor. To open the close value editor, select *Close Value Editor...* from the *File* menu. The close value editor is shown in figure 6.

The close value editor allows you to see and change all the close values at once. First you will want to change all the close values to your liking. The four buttons perform the following operations:

• Cancel will leave the close value editor without change the close-to values in memory or on disk.

• Revert will reset the close values on the screen to what they were when the program was first started.

• Temp will save the close-to values to memory, but not to disk.

• Save will save the close-to values to memory and to disk.

By saving close-to values to disk, you permanently change them. Whenever you start MacChemtab those values are read into memory.

By saving the close-to values to memory only, they are changed for the current execution of the program. Once you quit, they disappear.

Close Value Editor

Atomic Number	5.000
Atomic Mass	10.000
Melting Temp	100.000
Boiling Temp	100.000
Ionization Energy	25.000
Electronegativity	0.200
Specific Heat	0.200
Density	0.500
Year of Discovery	50.000
Atomic Radius	0.200
Valence Electrons	1.000
Family	1.000
Row	1.000

SAVE will save the values to disk

TEMP will save the values in memory during this session only

[Save]

[Temp] [Revert]

[Cancel]

REVERT will restore the original close values

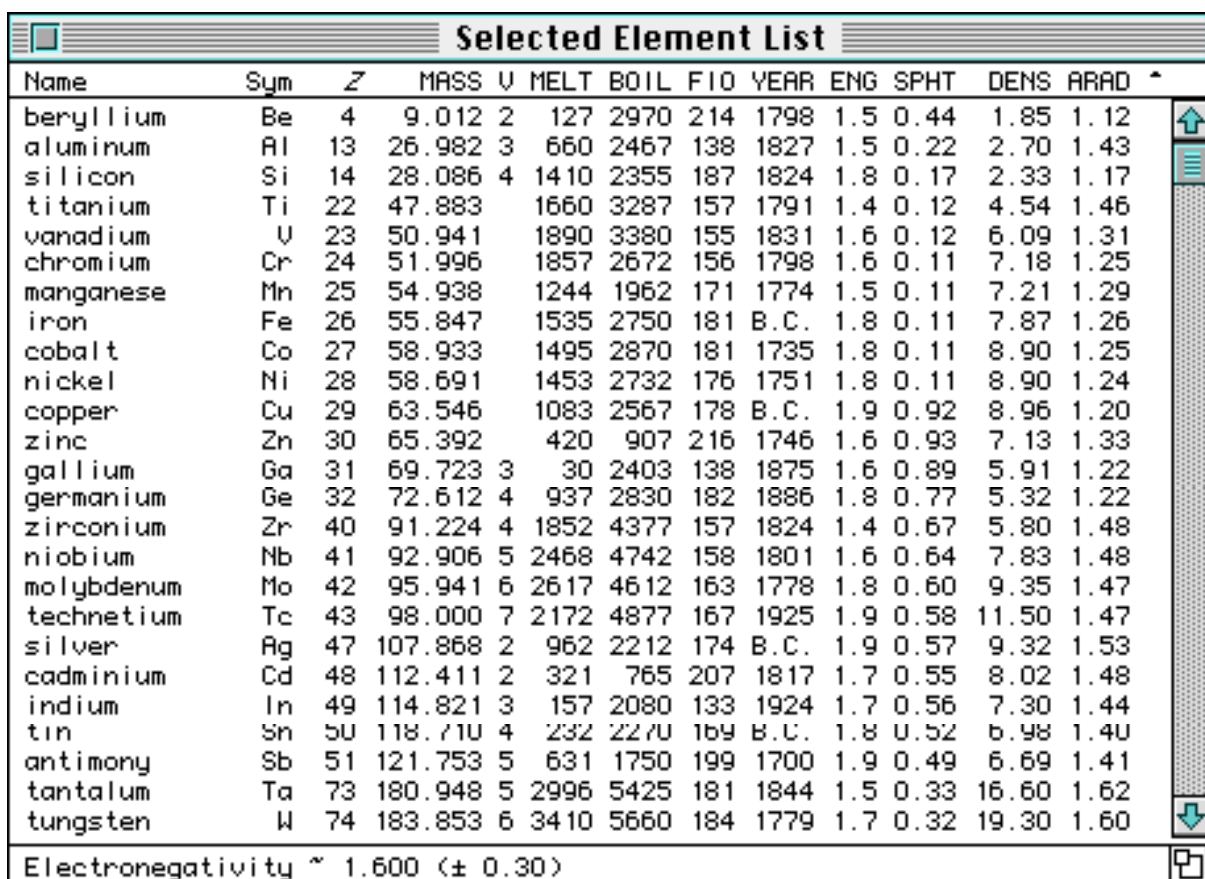CANCEL will leave everything unchanged

Figure 6

<u>Viewing Element Groups</u>

After you create a few search parameters, you may want to display the elements that meet your search parameters in a couple different ways. Each section below describes a different way to view this data.

The Element List

A list is one of the most common ways to view data. The MacChemtab list window has a variety of features that enable you to manipulate the data so that you can see some patterns more clearly. If you select *Selection List* from the *View* menu, you will see a window similar to the one in figure 7. If the menu is grayed out, or not selectable, it is because you have not created any search parameters. Read section 3 of this manual to learn how to create search parameters.

Name	Sym	Z	MASS	V	MELT	BOIL	FIO	YEAR	ENG	SPHT	DENS	ARAD
beryllium	Be	4	9.012	2	127	2970	214	1798	1.5	0.44	1.85	1.12
aluminum	Al	13	26.982	3	660	2467	138	1827	1.5	0.22	2.70	1.43
silicon	Si	14	28.086	4	1410	2355	187	1824	1.8	0.17	2.33	1.17
titanium	Ti	22	47.883		1660	3287	157	1791	1.4	0.12	4.54	1.46
vanadium	V	23	50.941		1890	3380	155	1831	1.6	0.12	6.09	1.31
chromium	Cr	24	51.996		1857	2672	156	1798	1.6	0.11	7.18	1.25
manganese	Mn	25	54.938		1244	1962	171	1774	1.5	0.11	7.21	1.29
iron	Fe	26	55.847		1535	2750	181	B.C.	1.8	0.11	7.87	1.26
cobalt	Co	27	58.933		1495	2870	181	1735	1.8	0.11	8.90	1.25
nickel	Ni	28	58.691		1453	2732	176	1751	1.8	0.11	8.90	1.24
copper	Cu	29	63.546		1083	2567	178	B.C.	1.9	0.92	8.96	1.20
zinc	Zn	30	65.392		420	907	216	1746	1.6	0.93	7.13	1.33
gallium	Ga	31	69.723	3	30	2403	138	1875	1.6	0.89	5.91	1.22
germanium	Ge	32	72.612	4	937	2830	182	1886	1.8	0.77	5.32	1.22
zirconium	Zr	40	91.224	4	1852	4377	157	1824	1.4	0.67	5.80	1.48
niobium	Nb	41	92.906	5	2468	4742	158	1801	1.6	0.64	7.83	1.48
molybdenum	Mo	42	95.941	6	2617	4612	163	1778	1.8	0.60	9.35	1.47
technetium	Tc	43	98.000	7	2172	4877	167	1925	1.9	0.58	11.50	1.47
silver	Ag	47	107.868	2	962	2212	174	B.C.	1.9	0.57	9.32	1.53
cadmium	Cd	48	112.411	2	321	765	207	1817	1.7	0.55	8.02	1.48
indium	In	49	114.821	3	157	2080	133	1924	1.7	0.56	7.30	1.44
tin	Sn	50	118.710	4	232	2270	169	B.C.	1.8	0.52	6.98	1.40
antimony	Sb	51	121.753	5	631	1750	199	1700	1.9	0.49	6.69	1.41
tantalum	Ta	73	180.948	5	2996	5425	181	1844	1.5	0.33	16.60	1.62
tungsten	W	74	183.853	6	3410	5660	184	1779	1.7	0.32	19.30	1.60

Electronegativity ~ 1.600 (± 0.30)

Figure 7

There are five distinct sections to the list window:

• The scroll bar enables you to scroll through the list of elements.

• The size box in the lower right-hand corner allows you to resize the window.

• The bottom of the screen lists the search parameters that were in effect when this window was created.

• The middle of the screen is a list of elements. By double-clicking on a list entry, you can pull up complete information about each listed element (see section 2, Viewing a Single Element).

• The top of the screen contains labels for each column. You will notice that one of the labels is italicized. This means the list you see is sorted by this characteristic. If you wish to change this, hold down the option key and click on the label you wish to sort by. The right-most label is an arrow that points up or down. This indicates that the sort is ascending or descending. You can change this by holding down the option key and clicking on the arrow. It will shift from up to down, or down to up and the list will update. Below is a listing of the labels and what they stand for:

Name - Atomic Name	Sym - Atomic Symbol
Z - Atomic Number	Mass - Atomic Mass
V - Valence Electrons	Melt - Melting Temperature
Boil - Boiling Temperature	FIO - First Ionization Energy
Year - Year of Discovery	ENG - Electronegativity
SPHT - Specific Heat	Dens - Density
ARAD - Atomic Radius	

The Periodic Table

Another good way to view patterns in the periodic table is to view the elements you have selected in the periodic table itself. To pull up a graphic of the periodic table, select *Periodic Table* from the *View* menu. This will create a window similar to the one in figure 8.
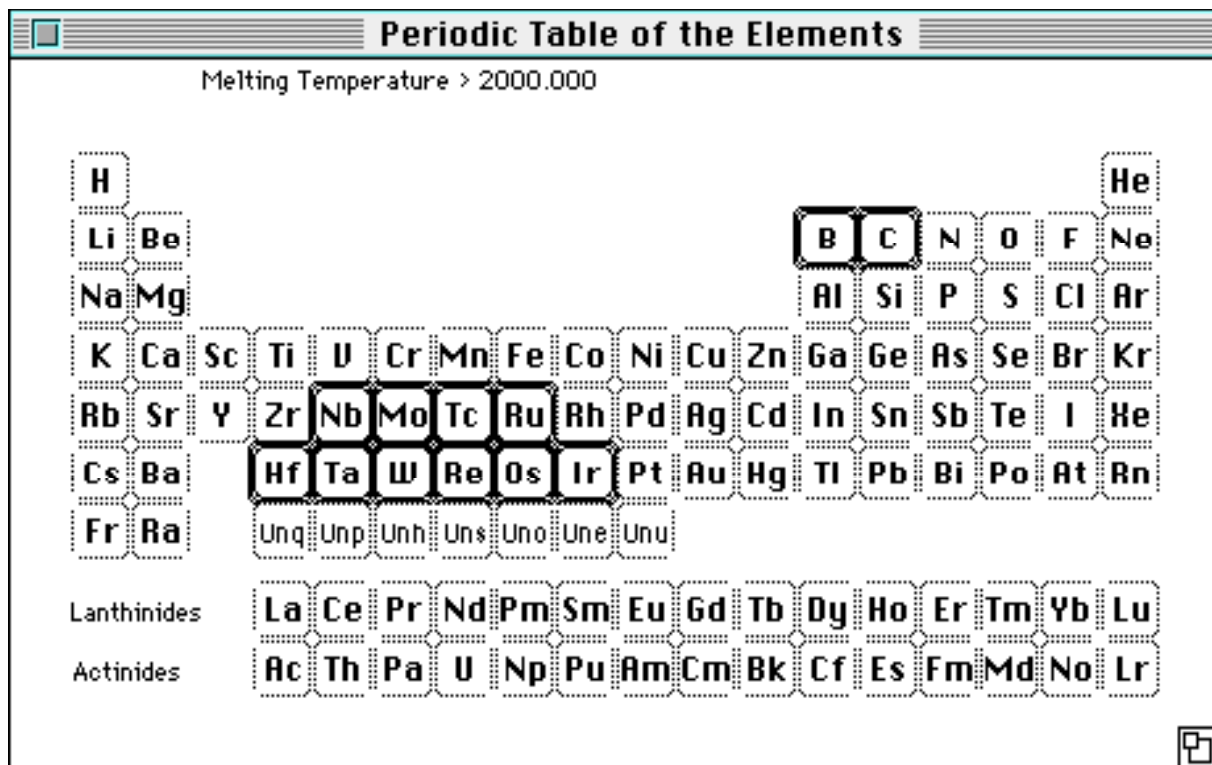
Figure 8

At the top of the window, your search parameters are listed. Each element that did not meet the search parameters is surrounded by a gray box. You cannot do anything with these. The elements that did meet your search parameters are surrounded with a black box. These are actually buttons that you can click in. If you do, you will see complete information about that element (see section 2, Viewing a Single Element).

<u>Graphs</u>

One of the best ways to see patterns is by using a graph. MacChemtab has a sophisticated graphing module built-in, and you can configure it to your liking. Note that under System 6 you cannot create color graphs.

Changing the Graphing Options

You can change all the graphing options by selecting *Set Graphing Options* from the *Graph* menu. You will see a dialog box similar to the one in figure 9.
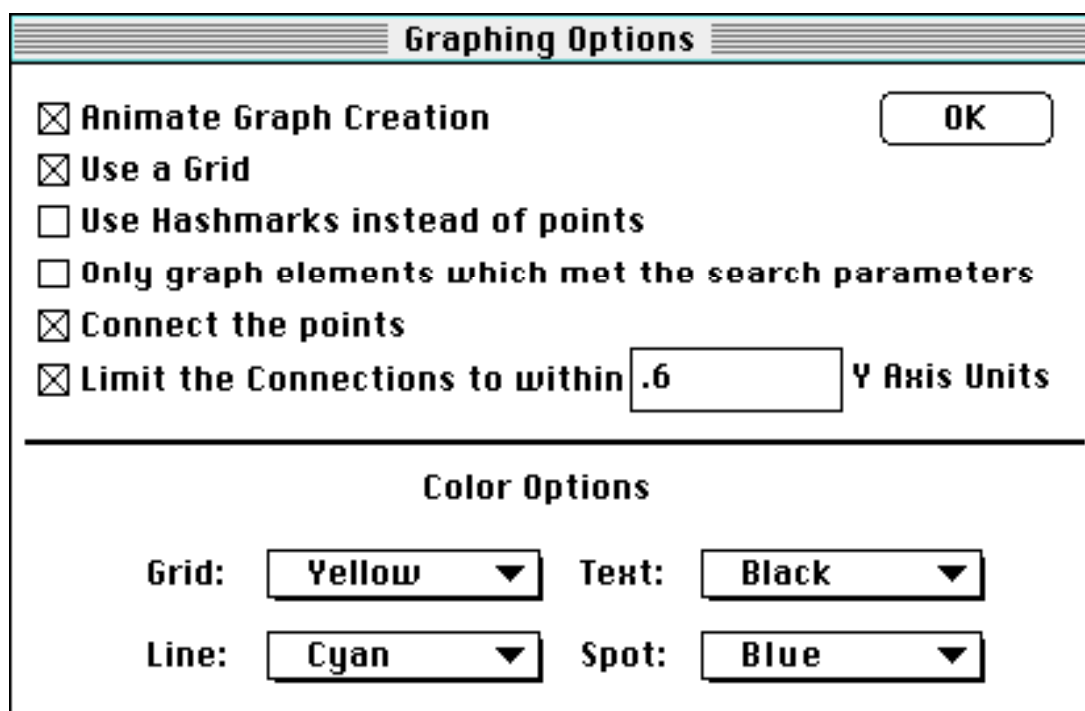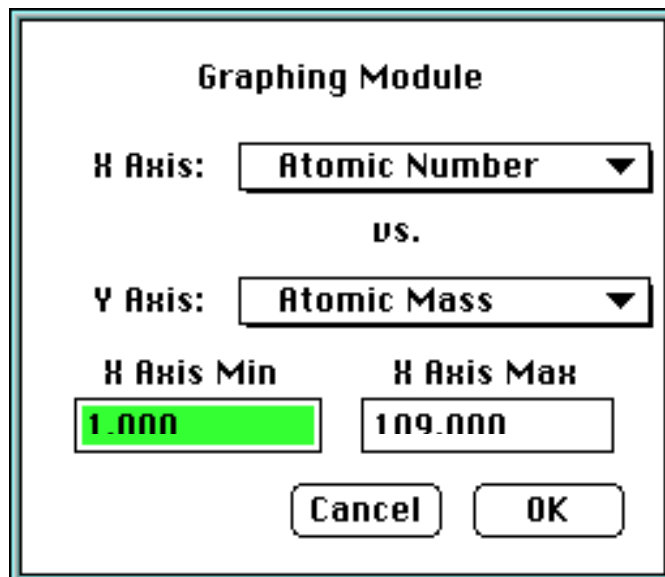

Figure 9

A description of each option is below:

• Animate Graph Creation - You have the option to see the graph while it is being created. If this box is checked, you will see each graph point displayed one at a time. If the box is not checked, MacChemtab will create the graph off-screen and copy it to the screen all at once.

- Use a Grid - You can have grid lines on the graph that extend across the graph from each label. Grid lines will appear only if this is turned on. If you are using System 7, you can change the color of the grid lines using the pop-up menu at the bottom of the dialog box. The pop-up menu will be grayed-out until *Use a Grid* is checked. Note that if the grid lines are yellow or white, they will not show up when printed.

- Use hashmarks instead of dots - You can have each point on the graph represented by a dot or by hashmarks. Dots will be displayed if this option is turned off.

- Use only elements which met the search parameters - If you wish, instead of using all the elements when creating a graph, you can use the elements that meet the search parameters you create. This way you can filter out any special elements from your graph. This option is only available when you have created some search parameters.

- Connect the points - If this option is on, each point on the graph will be connected by a line.

- Limit the connection spacing to... - If this option is on, and the proper value is placed in the text-box, you can eliminate unnecessary lines on the graph. A good example of this option is to graph Atomic Number on the X axis, Electronegativity on the Y axis, and limit the connection spacing to .6. This will eliminate lines that would be drawn between elements on opposite sides of the periodic table. The result is the same as removing the vertical lines from a graph of y=tan(x) on a computer. The computer cannot tell the difference from one end of the tangent line from the other, so it connects them. Since this line does not actually exist, it should be removed. By removing unnecessary lines from a graph, you get rid of extra information that may distort your perception of a pattern.

- The pop-up menus at the bottom allow you to change the colors used on different parts of the graph. These are only available for users with System 7.

- Click on the OK button to accept the options. There is no cancel

button.

Creating a Graph

After you customize the graphing options as described above, you must set the characteristics that will lie on each axis of the graph. To do this, select *Graph* from the *Graph* menu. You will see a dialog box similar to the one in figure 10.

Figure 10

To choose the characteristic for each axis, use the pop-up menus. At the bottom of the dialog box are two numbers labeled, X Axis Min and X Axis Max. The values that appear in these boxes represent the maximum values for the elements you are going to graph. In this example, you are going to graph all the elements with an atomic number between 1 and 109. You can change these values by typing in new ones. For example, if you only want to see elements past number 50, type 50 into the X Axis Min box.

Click Cancel to cancel this operation or click OK to create a graph. The graph will look similar to the one in figure 11.
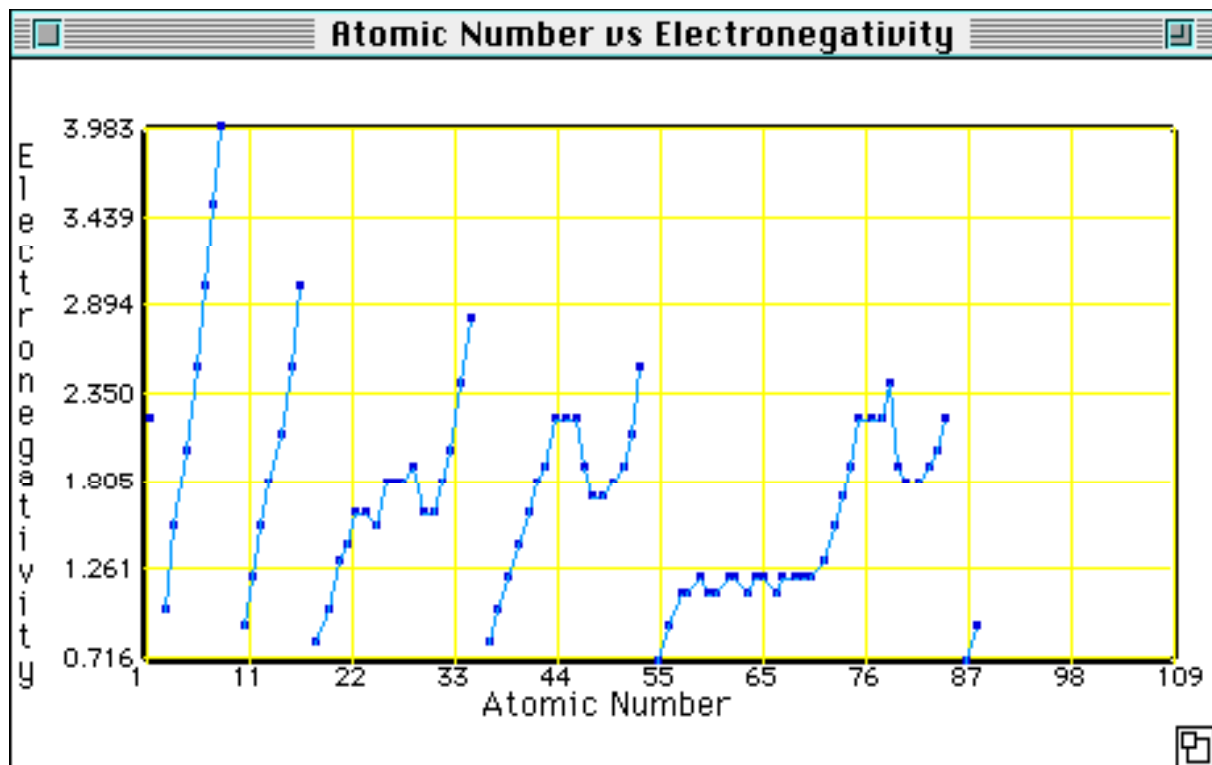
Figure 11

There are two things you can do with the graph window. You can resize the window, and the Macintosh will shrink or expand the picture to fill up the entire window. You can also click on any graph point to bring up complete information about that particular element (see section 2, Viewing a Single Element).

Window Operations

Open and Save

At some point you may want to save a window for later reference. To do this, select *Save As...* from the *File* menu when the window you wish to save in the front-most window. You will be prompted as to where you wish the saved file to go, and what name to give it. MacChemtab uses the standard file dialog to do this, and it is something you should already be familiar with. Figure 12 shows a Save File dialog box, and Figure 13 shows an Open File dialog box.
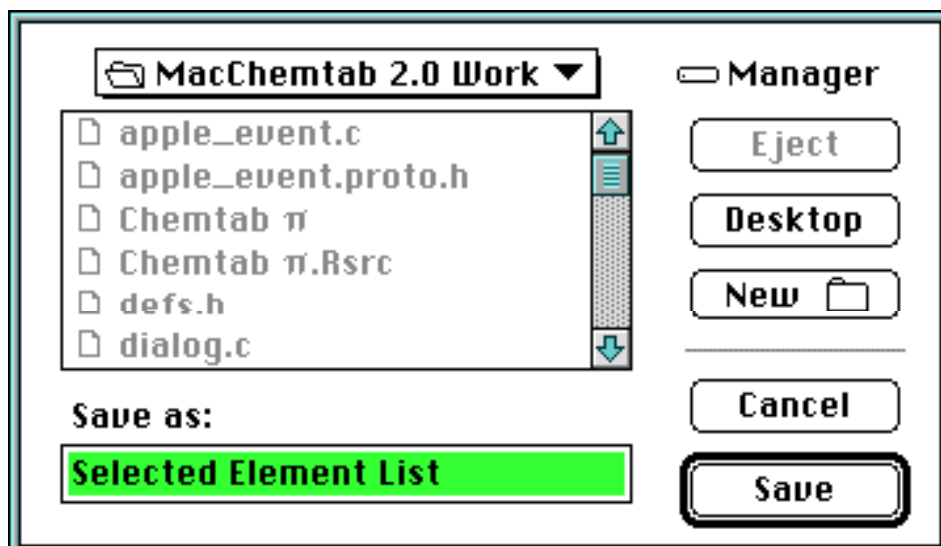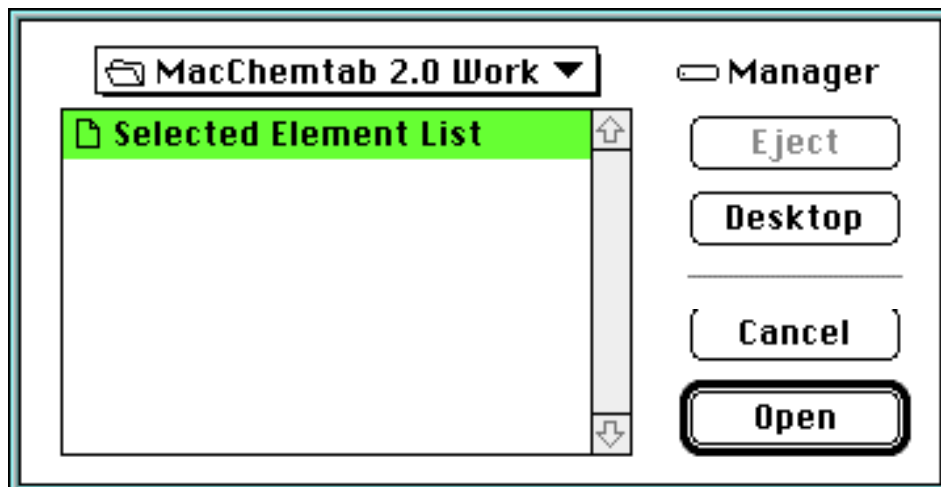

Figure 12

Figure 13

Close / Close All

You can close a window in one of three ways. You can click on the close box for the window, which will make the window close. You can select *Close* from the *File* menu to close the front-most window, or you can select *Close* All from the *File* menu to close all of MacChemtab's open windows.

Print

You can print any window MacChemtab creates, except for an element list window, by selecting *Print* from the *File* menu. MacChemtab uses the standard system printer driver that you are probably already familiar with. You cannot print an element list window because that function has not yet been implemented into MacChemtab 2.0. **NOTE!** You can only print to a LaserWriter or StyleWriter printer. Printing is not available to ImageWriters as far as I know.. but you could try it..