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Copyright Notice

ChemPen+.

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Introduction

ChemPen+ is designed to let chemists, chemistry students or chemical workers illustrate chemistry documentation. With **ChemPen+** you easily create diagrams like **Figure 1**. **Figure 1**

ChemPen+ was designed to be simple, intuitive and versatile. Drawings are created using menus, mouse clicks and drags. Special **editing tools** further simplify drawing. **ChemPen+** is chemical aware. That is, the program tries to keep your structures chemically accurate.

ChemPen+ drawings can be copied and pasted into popular Windows word processors and graphics applications. However **ChemPen+** is not just a drawing program. **ChemPen+** is extensible. Special libraries are under development that will allow ChemPen+ to do special chemical calculations. For example a special C-13 NMR library is available to users now.

Next

Figure 1

Introduction - 2

It helps to know a little about **ChemPen+'** internal workings. **ChemPen+** uses atom, bond, structure, symbol and label objects to create drawings. Atoms and bonds, the most basic elements, are used to create the other objects. **ChemPen+** combines these objects to create a drawing.

Groups are collections of atoms and bonds such as t-butyl. **Rings** are a special class of groups. When groups are created they are added to a group list. This makes selecting them for editing easier. A structure created by **cloning** an selected group of atoms and bonds is added to the drawing as a new group.

ChemPen+ drawings can be annotated with special atoms called **Labels**. Labels are added and edited with the **Text Editor**

Arrows and arcs are examples of **Symbols**. Symbols are added from the **Symbol Menu**. Symbols are edited with a special **Symbol Editor**. As **ChemPen+** is improved, more symbols will be added.

Next

A copy or duplicate

Introduction - 3

Drawing with ChemPen+ is done with menus and <u>editors</u>. Editors activate only if their targets are present. The area where the drawing is displayed is referred to as the **Pad**. Vertical and horizontal scrollers let the user shift the drawing up, down, left and right. Up, down, left and right movement can also be done with the arrow keys.

To illustrate the drawing process <u>Figure 1</u> is drawn. In each step the <u>bold colored</u> words state the result of each step. The actions to perform each step follow. Menu commands or button commands are in **bold** letters.

Equivalent keyboard commands, if available, are revealed when you click on these letters. Target atoms, bonds, groups and symbols for each action are highlighted in red.

Undo and **Redo** restore a drawing to the its state prior to a drawing operation. Each of the **editors** has an **Undo** button to undo the last editing operation.

Click **Tutorial** for to learn how to draw with **ChemPen+**

Drawing with ChemPen+ - Step 1

This tutorial will get you started using **ChemPen+** by illustrating the drawing process with an example. Most of the drawing is done with menus and where equivalent keyboard commands are available they are revealed if you click on the sequences of menu commands.

In some steps the target of an action is highlighted in red. This is the target, and the illustrated structure is the *result* of the action.

Add a cyclohexane ring

From the main menu select **Ring**, **Add**, **6** then click near the left side of the Pad.

Result



Next Step

Drawing-Step 2
Fuse a second cylclohexane to the right side bond of the first.
From the main menu select Ring, Fuse, 6 and click near to the right of the highlighted target bond.

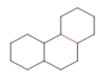
Result



Next Step Previous Step

Drawing - Step 3
Repeat the previous step fusing a third cyclohexane to the highlighted bond.
Click above and right of the highlighted target bond to fuse another ring.

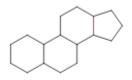
Result



Next Step

Drawing - Step 4
Fuse a cyclopentyl ring to rightmost bond in the previous structure
Select Ring | Fuse | 5 and click near the target bond.

Result



Next Step

Drawing - Step 5

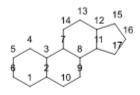
Number the Structure-This optional step is just to make the next step easier to explain

1. Start above left of the structure and drag the mouse until the blue rectangle surrounds the

structure. The group is highlighted and the **Group Editor** activates.

2. Click the **On** button in the **Numbers** box.

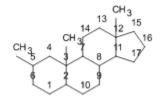
Result



Next Step

Drawing - Step 6 Branch methyls from the previous structure and turn off numbering 1. From the main menu select **Bond | CH3**and near atoms 3, 5, and 12 2. Click **Reset** to stop branching.

Result



Next Step

<u>Drawing - Step 7a</u> <u>Convert diagonal branch to OH</u>

- 1. Click the *right* button near the #5 **CH3.** The **Atom Editor** is activated.
- 2. From the Atom Editor Menu select Atom | Non-Metals | O. The CH3 changes to O.
- 2 On the periodic table click **O.** The **CH3** changes to **OH**3. Select the structure. Click the **Numbers Off** button.

Result

Next Step

Drawing - Step 7b.

- Select the **Reverse** button to change **OH** to **HO**.
 Click the Atom Editor **OK** button.
- 3. Select the entire group and click the **Numbers Off** button on the **Group Editor**
- 4. Click the Group Editor **OK** button

Result

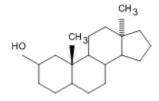
Next Step

Drawing - Step 8a

Modify the Methyl bonds

- Hold **Shift** and click the right mouse button near the right hand methyl.
 The **Bond Editor** activates
- 2. Click the **In | Out** button until an out bond is formed.
- 3. Click near the right methyl bond and change it to a hatched bond with the **In | Out** button.
- 4. Click the **OK** button.

Result



Next Step

- Drawing Step 8b
 Clone the Group
 1. Select the entire group thus activating the
 2. Click the Clone button.

 Group Editor
- 3. Click the **OK** button.

Result

Next Step

- Drawing Step 9
 Create a carbonyl and a double bond
 1. Hold shift and click near the right structure's OH. The <u>Bond Editor</u> activates.
- 2. Click the **double** button to create a carbonyl.
- 3. Click the highlighted bond in the right structure and click the **double** button.
- 4. Click the **OK** button.

Result

Next Step

Drawing - Step 10

Add and modify an arrow

- 1. Select Symbol | Arrows | choicefrom the Symbol Menu where choice one of the arrows pictured in the sub menu.
- 2. Click between the two structures to place the arrow.
- 3. Click near the head or tail of the arrow. The symbol editor is activated.
- 4. Click +50% to increase the size by 50%.5. Click the Style button until the arrow changes to the appearance below.
- 6. Click the **OK** button.

Result

Next Step

<u>Drawing - Step 11</u> Add a label

- 1. Select **Label** from the main menu.
- 2. Click just above the arrow. The word label appears and the label editor activates.
- 3. Select the word label and type oxidation
- 4. Hit **Enter** or the **OK** button.

Result - The drawing is done!

Symbol Menu

Arrows, arcs and triangles are added from the symbol menu. As ChemPen+ develops and based on customer demand other symbols will be added.



Menu Commands

All drawing is done from the Main Menu shown below.



FileLinkAlkaneResetAtomsRingBranchSymbolBenzeneSymbol|Te

Benzene Symbol|Text
Font Undo/Redo

Using the Keyboard

Besides entering and editing text the keyboard can be used to navigate **ChemPen+**. All keyboard commands move the drawing while not the scrollers remain unchanged. The keystrokes that apply to **ChemPen+** are defined below.

Tab - moves the drawing right 1/8th the Pad width.

Arrow keys- the up and down arrow keys move the drawing up or down by 1/8th the Pad height. The left and right arrow keys move the drawing left or right by 1/8th the Pad width.

Page Up, Page Down - the page up and down move the drawing up and down respectively by one page height

Also see: Entering and Editing Text

Overview of Editing

ChemPen+ editing is done with the editing tools listed below. Each editing tool is activated either by selecting a target atom, bond, group, symbol or label. Selecting the object activates its applicable editor. Each ChemPen+ editor is listed below.

Atom Editor

Bond Editor

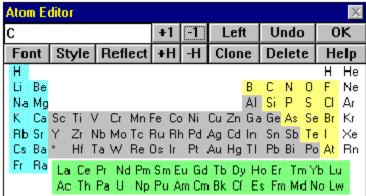
Group or Ring

Symbol

Text Editor

Also see Introduction

Editing Atoms



Use the Atom Editor's buttons, menus and text editor to change the currently selected atom.

To Activate the Atom Editor:

- 1. Right mouse button click near the target atom or
- 2. Select **Edit|Atom** and click near the target atom.

Also see Editing ,Menu Commands

The selected atom can be changed by clicking thean atom on the periodic table. By default carbons are shown as points. Explicit hydrogens are shown on other non-metals by default. Edit the atom's symbol string using the text box

Launches the font dialog box letting you change the atom's font

Increments or decrements charge of atom. If atom is a non metal hydrogens are added.

Changes atom symbol style. Toggles between explicit H's, hidden Hs and hidden.

Reflects and reverses the order of the string characters in the text box.

Shifts text left or right

Duplicates the atom

Deletes the atom and cuts attached bonds.

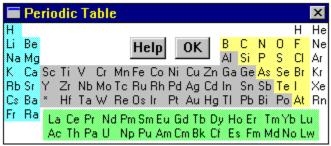
Undoes atom editing

Adding an AtomClick on the atom you want to add then click on the pad to add the atom

Atom Menu

Activates periodic table

To add an atom click its symbol on the periodic table then click the location on the pad where the atom is to be added.



Also see: Menu Commands

Branch

The group menu is used to **branch** groups from an existing group or to **link** two atoms.

									_
<u>B</u> ranch	ΑΙ <u>κ</u>	gane	Ben <u>z</u> e	ne	<u>R</u> ing	<u>Ѕ</u> уп	nbol	<u>T</u> ext	<u>H</u> elj
bond	NH2		12		CH2OH		NCO		
CH3		PH2			СНО		N02		
Н		SH	ı		CN		N	103	
F		=C	H2		CH=CH2	2	0	CH3	
ОН		=0	1		COCH3		S	O3H	
CI		=N	IH		CONH2		S	O2NH2	
Br		=N	ЮН		COOH		S	02	
I		=N	I=0						

Alkane Menu

Alkanes are **added** to the drawing or **branched** from existing atoms by selecting them from the alkane menu. The number is the length of the linear chain. T-butyl can be added. T-butyl, i-propyl and vinyl can be branched.



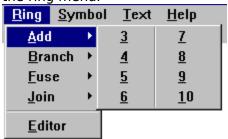
Benzene Menu

Benzene can be **added** to the pad, **branched** to an existing atom or **fused** to an existing bond by selecting the appropriate item on the benzene menu.

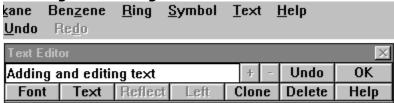


Ring Menu

Rings are **added** to the pad, **branched** from existing atoms or **fused** to existing bonds by selecting the appropriate item on the ring menu.



Entering and Editing Labels



Adding and editing text

Text labels are entered and edited with the **text editor**. The text editor is just the atom editor with some features disabled. Clicking an atom when the text editor is active activates its other features. To enter a label click **Label** in the main menu and click the location on the Pad where to place the text. Text is entered in the text window. A blinking caret appears where the text will be entered and typed text appears as red on the Pad.

Reset

Turns off drawing command repetition. If a drawing command is invoked, repeated clicking on the Pad will repeat the operation until **Reset** is pressed. **Reset** is grayed when inactive. Selection of another menu command replaces the currently active drawing command.

Undo and Reset

Undo reverses the most recent drawing command. Undo does not correct the very first drawing action as this can be undone by using **File | New. Undo** can be undone with the **Redo** command.

Label Font

Opens a font choosing dialog allowing the user to change the label's font.

Label TextToggles the labels font between regular, *italic*, **bold**, and *bold italic*.

Text Box

Use the text box to enter or edit a label's text.

Label Undo

Restores selected label to pre edited condition.

Delete

Deletes the Label.

Clone

Creates a duplicate of the label and puts it in the Pad's upper left corner.

OK

Press OK when done

Entering and Editing Formulas

The text editor is used to enter or modify an atom's text. Text entered in this window is formatted into molecular formula format. Pluses(+) and minuses(-) are treated as charges and are made superscripts. Numbers are converted to subscripts. In future versions of ChemPen+ will implement more sophisticated treatments of the text.

Atom Editor - Font ButtonUse the **Font** button to open the font selection dialog and to change the font of the selected atom or label fonts.

Atom Editor - Reverse Text

Use the **Reflect** button to reverse the order of the characters in a symbol or molecular formula.

Atom Left/Right Button
Use the Left/Right to shift the atom's text left or right. The button's title changes according to the condition of the specific atom selected

Atom Style Button

Use the **Style** button to change the style of an atom. The button's title toggles between the various styles, e.g. **C,** or **CH3**, available to a given atom. The numbers and types of styles will change as **ChemPen+** evolves.

Atom Delete Button

Use the **Delete** button to delete an atom and its attached bonds.

Atom Undo Button Use the **Undo** button to undo any change.

Atom Editor - OKUse the **OK** button to close the editor and accept the editing changes.

Atom Editor -Text Box

Enter formulas or enter text for atoms or labels into the Atom Editor Text box. Text is entered by normal typing. For atoms the current implementation of **ChemPen+** treats characters as follows. Numbers become subscripts. Pluses(+) and minuses(-) become superscripts. Letters are unaffected.

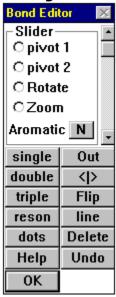
For Labels all characters are treated the same.

Atom Editor Help ButtonDisplays the Help topic for this button.

Atom Editor Clone Button

Duplicates the currently selected atom or label and puts the copy in the upper left corner of the Pad.

Editing Bonds



The bond editor tool is used change the character and appearance do bonds. To activate the bond editor do one of the following.

To Activate the Bond Editor

Select a bond with Ctrl | R Mouse Button or

Click **bond | Editor** and click near the bond to be edited **or**

Click **Edit | bond** and click near the bond to be edited.

Also see **Editing**, **Menu Commands**

The bond editor slider pivots, rotates or zooms the selected bond depending on the setting of the radiobuttons.

single - changes a bond to a single bond

double- changes bond to a double bond.

triple - changes bond to a triple bond.

resonance - changes bond to double bond with one dotted line

dots - changes bond to a dottet line such as in a hydrogen bond.

Out - toggles the bond between out, in and in the plane.

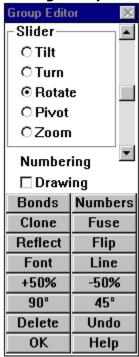
- shifts a multiple bond left or right.

Flip - exchanges the head of an out pointing bond.

Line - changes the line thickeness.

Delete - deletes the bond and saturates its atoms.

Editing Groups and Rings



Use the Group Editor tool to edit rings and other structures. To activate the **Group Editor** select a group by click **Ctrl | right mouse button** near the target ring or group. Alternatively, select a group of atoms by dragging the mouse until the atoms are surrounded by the blue rectangle. Click each part of the **Group Editor** to learn its function.

Also see Editing ,Menu Commands

X, Y, Z, Pivot, Zoom
Use the slider to Rotate. Pivot or Zoom the structure. X, Y and Z radio buttons select the rotation axis. Pivoting occurs around the Z axis.

Numbering

Determines basis of numbering. When **Drawing** is checked numbering starts at one plus the highest number of an already numbered atom. When **Drawing** is unchecked numbering starts at 1.

Bonds button

The bonds button shifts all of the multiple bonds in a group left or right toggling between styles below.



Line button

The line button toggles between line thicknesses of **0**, **1** and **2**. Thickness 0 and 1 are the same until pasted into another application as a picture where a thickness of 1 changes with zoom while a thickness of 0 remains constant.

±50% Zoom

Enlarges or shrinks the group by a one time 50%.

Font button

Font launches the font dialog which allows the user to change the font of the selected group.

Group FuseCombines selected atoms and bonds into a new group that can be selected with the control right mouse button.

Numbers button

Use the **Numbers** button to number the selected atoms. If the **Group** box is checked numbering starts from 1 with respect to the group. If **Drawing** is

A selected group of atoms can be numbered by selecting **Numbers**. If the **Group** box is checked and **Drawing** unchecked the numbering starts at **1**. If **Drawing** and **Group** are checked, numbering runs from the highest number of any previously numbered group in the drawing plus **1**. Any other combination of checks results in no numbering.

Reflect/Flip buttons
Reflect replaces the structure with its mirror image. Flip replaces its image with its upside down image.

Group Editor Buttons

Clone creates a saturated duplicate of the selected group.

Fuse combines the selected atoms and bonds into a new group

Reflect reflects structure through its vertical axis.

Flip flips structure about its horizontal axis.

+50%, -50% zooms structure by amounts indicate

+900, -900 rotates structure by 1/4th turn.

+450, -450 rotates structure by 1/8th turn.

Delete, Undo delete structure or undo all editing.

Delete and Undo

Delete deletes a group and all bonds connecting it to non selected atoms. Undo undoes all editing since group editor was started.

Note: The group editor will not delete labels or symbols.

Numbers turns group numbering on or off

Clone

Creates a duplicate of the selected group. If the selector cuts into bonds they are cut and replaced by implicit hydrogens.

Note: This group editor button does not clone labels or symbols.

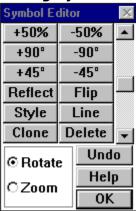
Numbering Check Box - determines if group numbering is relative to the selected group or the entire drawing.

Rotate 90o or 45o

Rotates tilts, turns or rotates the group by 90 degrees or 45 degrees depending on which slider function is selected. Has no effect when pivot or zoom is selected.

 $\ensuremath{\mathbf{OK}}$ saves the edited structure and closes the group editor.

Editing Symbols



Use the symbol editing tool to edit symbols such as arrows and arcs. To activate the **Symbol Editor** click the **Right Mouse Button** with the cursor near the target symbol. Alternatively from the main menu click **Symbol** | **Editor** and click near the target symbol. Click each part of the illustration in this figure to learn its function.

Also see Editing

Symbol Editor Buttons

Reflect and **Flip** are inactive

900,-900,

+450,-450 rotate the symbol by the amount shown. +50%, -50% zooms the symbol by the amount shown

line changes the line thickness

affect depends on the symbol Style's

Clone creates a duplicate of the selected symbol

Delete deletes the selected symbol

Symbol Editor Radio ButtonsThe radio buttons determine the function of the slider namely **Zoom** or **Rotate**

Symbol Editor SliderThe slider rotates or zooms the symbols depending on the setting of the radio buttons.

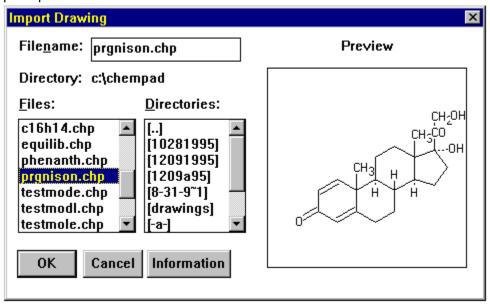


Opening, saving and exchanging **ChemPen+** drawings is done, from the **File Menu.** Click on a menu item to learn its function

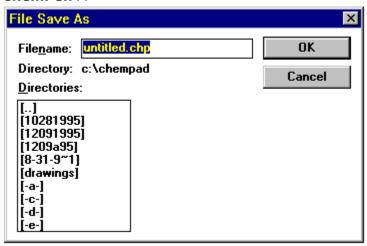
Also see Menu Commands

File New erases the current drawing, if any and starts a new drawing. If there is a drawing on the Pad you are prompted to confirm the operation. The new drawing is given the file name **untitled.chp**.

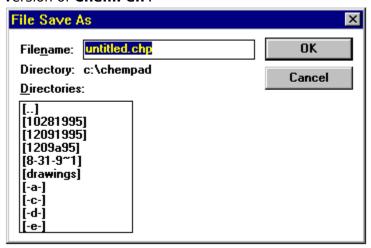
File Open executes the **file open dialog** below. The **Preview** window lets you see a scaled down view of the selected file. The **information** button will display any information entered by the creator. Click each part of the figure to learn its function. If you click the **OK** button the previewed drawing replaces the current drawing on the pad, if any. If the Pad contains a drawing you are prompted to erase it and load a file.



File Save excutes the file save dialog if the name of the file drawing is untitled. **Ok** saves the drawing to disk. If the filename already exists you are prompted to confirm the saving. File Save is inactive in the demo. version of **ChemPen+**.

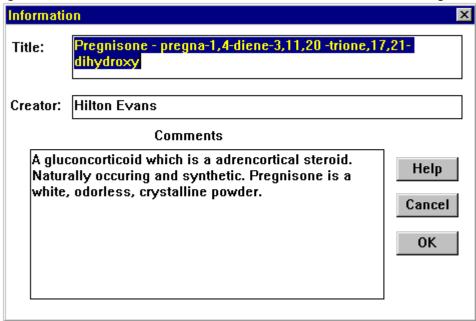


File SaveAs prompts you for a file name, even if the drawing has been given a filename, and saves the drawing to disk. If the filename already exists, you are prompted to confirm the save. SaveAs is deactivated in the demo. version of **ChemPen+**



File Information executes the file information dialog

Use the dialog to the name of the drawing, the name of the creator and to add eight lines of comments. The information is saved with the drawing



File Copy

Copy puts a **bit map** or **metafile** image of the drawing on the Clipboard that can be pasted into another application. Metafiles, which often appear on the clipboard as pictures, in general give better quality printed and displayed images than bit maps. Bit maps are included for applications that don't accept Metafiles.

Bit Maps

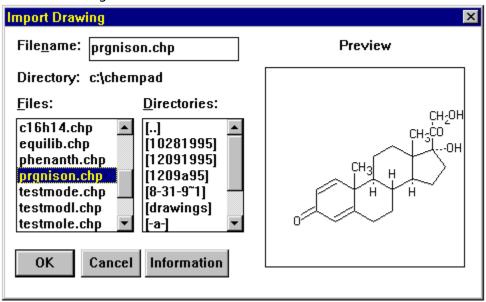
Bit maps are raster representations of pictures. **ChemPen+** copies its drawings to the clipboard in metafile or bit map format. Because of their larger file size and poorer scaling characteristics, betimes should only be used when the pasted to application requires them.

Metafiles

Metafiles are special sets of instructions that represent a drawing a set of commands. **ChemPen+** copies drawings to the clipboard in metafile or bit map format. Because of their relative device independence and generally smaller size Metafiles are the preferred **ChemPen+** drawing format to copy to the clipboard.

File Import

File Import opens the **file open dialog** and lets you load a drawing without erasing the present drawing. The new drawing is inserted to the right of the current drawing.



File Configure

Use **Configure** to set **line**, the default line width; **path**; **font**; and **bond** the default bond length. The size of the jump that occurs when a drawing or structure is moved with the arrow keys can also be changed from this menu. For programs with NMR libraries NMR nuclei can be selected from here. The information is saved in file named **!ChemPen.cfg**. If **!ChemPen.cfg** is found in the same directory as **ChemPen.exe**, the drawing is initialized with the **! ChemPen.cfg** data. If **!ChemPen.cfg** is not in **ChemPen+**'s directory then it's created upon starting **ChemPen+**.

File Exit

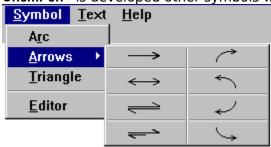
Shuts down the application. If a drawing exists you are prompted to save it.

Loading and Importing DrawingsUse the **File Open/Import dialog** to load existing drawings

Label

Adds a label to the drawing and activates the $\underline{\textbf{label editor}}$.

Symbol



Atom

Adds an atom to the drawing. Also launches the ${\color{red} \underline{\textbf{Atom Editor}}}$

branch

Branches a single bond or links to atoms. If **Branch** or **CH3** is selected, clicking near an atom forms branches until **Reset** is selected or a different menu item is selected. If **Link** is chosen clicking twice near two different atoms will form a single bond. Repeated selection of pairs of atoms bonds them until **Reset** is selected.

Note: no link occurs if either atom's valence is exceeded.

Also see: Editing Bonds

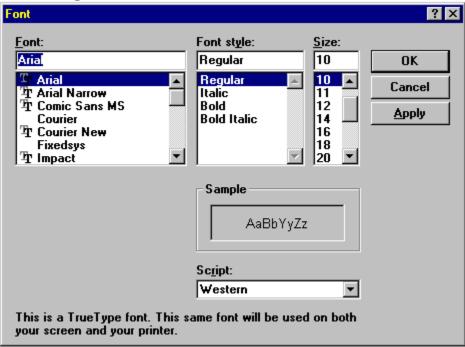
Ring

Adds, branches, links or fuses a ring to an existing structure. If **Add** is chosen a ring is drawn centered at the point on the drawing where the mouse is clicked. If **Branch** is selected, clicking near an atom branches from that atom. Branching occurs if the valence of the target atom is not exceeded. If **Fuse** is selected, clicking near a bond fuses the ring to that bond. The ring will not be fused if the valence of the atoms will be exceeded. If **Join** is selected, clicking near an atom joins an apex of the selected ring to the target atom. The ring is joined if the valence is not exceeded.

Font

Launches the **font dialog** that allows the user to change the current drawing font. The font is in effect until the application is closed.

Font Dialog



Link

To form a new bond between two existing atoms select link then click near each of the two atoms. Use **RESET** to stop linking.

Special Menu
The special menu provides access to libraries and options that extend ChemPen+' functionality. All versions of ChemPen+ come with a molecular weight calculator under the special menu. When an extension is added its selection appears in the special menu.

Using the Mouse

ChemPen+ uses the mouse in several ways to simplify work. Combining the shift and control keys with the right mouse button have special functions in **ChemPen+**.

Clicking the **right mouse button** - selects the nearest atom or symbol and activates the **Atom Editor** or the **Symbol Editor**

Holding **Shift** and clicking the **right mouse button** - selects the nearest **bond** and activates the **bond editor**

Holding **Ctrl** while clicking the **right mouse button** - selects the nearest **ring** or **group** and activates the **Group Editor**.

Dragging the mouse from <u>above and left</u> of any group of atoms to <u>below and right</u> of the atoms and combines them into a group activating the <u>Group</u> <u>Editor</u>. The selected group is highlighted.

Also see Editing

Customer Support

Customer Support for ChemPen+ is available to registered users via America On-line, via Internet mail or by US Mail. If you have a question, want to report a bug or have a problem with ChemPen+write to the following. For registered copies be sure to include your registration number in any correspondence.

America Online: HFEvans

Compuserve: 102303.2120

Internet Mail: HFEvans@AOL.com

102303.2120@Compuserve.com

U.S. Mail: Hilton Evans

232 Canton Street#312 Randolph, MA 02368