Copyright Notice

Installing ChemPen3D

Windows 95

1. Make a backup copy of the ChemPen3D Disk
2. Insert the disk into floppy drive A:
3. Double Click the 'My Computer' Icon
4. Double Click the Floppy Disk Icon
5. Double Click Setup.exe
6. Follow the instructions

Windows 3.x

1. Make a backup copy of the ChemPen3D Disk
2. Insert the disk into floppy drive A:
3. Run the File Manager
4. Select File | Run ... and in the text box type A: Install and type Enter
5. Follow the instructions
6. Wait until you are prompted for the Installation Complete Message

Unlocking ChemPen3D

ChemPen3D must be unlocked to save or print drawings; although you can copy it to the Windows® clipboard. An **Unlock** code is supplied when you purchase **ChemPen3D.** If you have a valid unlock code, enter your *first name, last name* and *unlock code*. All three must be entered to unlock the program. If you have need a code click **how to register ChemPen**.

Introduction

ChemPen3D combines chemical structure drawing and molecular mechanics in one software application. **ChemPen3D** simplifies the illustration of chemistry documentation for chemists, chemistry educators, students and chemical workers. With **ChemPen3D** you easily create diagrams like the drawing in **Figure 1a.**

However **ChemPen3D** is not just a drawing program. **ChemPen3D** is also a basic molecular mechanics modeling program . **ChemPen3D** uses an extended version of the popular **DREIDING** molecular mechanics force field to compute molecular geometries. Thus you can create structures such as that in **Figure 1b.**

By combining the DREIDING force field a partition function **ChemPen3D's reaction tool** lets the user build and analyze the energetics of chemical reactions. With the **Measurement Tool** bond lengths, bond angles torsion angles and interatomic distances can be displayed.

Figure 1a

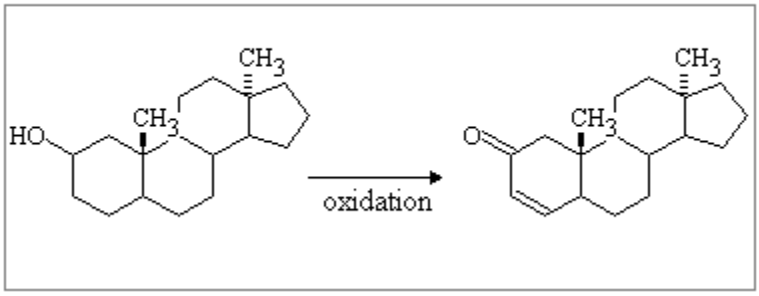
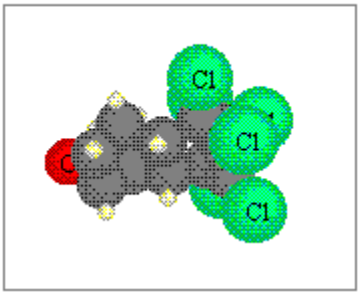


Figure 1b



Next

Introduction cont'd

ChemPen3D is intuitive. Drawings is done with menus and mouse clicks. **Special Editors** further simplify drawing. **ChemPen3D** is chemical aware. That is, the program tries to keep your structures chemically accurate.

ChemPen3D drawings can be printed or pasted into popular Windows word processors and graphics applications. **ChemPen3D** 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. **ChemPen3D** combines these objects to create a drawing.

Groups, such as t-butyl and CONH2, are collections of atoms and bonds. **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.

Simple text is added as **Labels**. A special type of label is the formula text. A formula has the format of a molecular formula but carries no chemical information. Labels are added from the **Symbol Palette** 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 **ChemPen3D** is improved, more symbols will be added.

Next

The ChemPen3D DREIDING Force Field

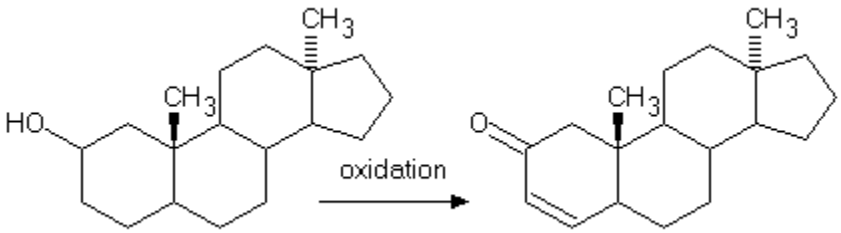
The DREIDING(1) force field was developed for calculating the geometries and dynamics of organic, biological and main group inorganic molecules with molecular molecular mechanics(2) methods. Compared with more specialized force fields, DREIDING, sacrifices a little geometrical accuracy in favor of treating a larger variety of molecules.

The original DREIDING field was parameterized for non metal elements and for Na, Ca, Zn and Fe. The **ChemPen3D** version of DREIDING is extended to include the entire Periodic Table. DREIDING uses *implicit* protons to greatly improve optimization speed . While molecules with explicit protons can also be optimized that is not usually necessary.

ChemPen3D handles the geometry of metal complexes. The **ChemPen3D** version of DREIDING tries to predict the hybridization of complexed transition metals based on oxidation number, base electronic configuration, and ligand number.

1) S.L. Mayo, B. D. Olafson, W. A. Goddard III, *J. Phys. Chem.*, 94, 8897(1990)
2a) N. L. Allinger, *J. Am. Chem. Soc.,* 99, 8127(1977)
2b) N.L. Allinger, Molecular Mechanics, Am. Chem. Soc.; Wash. DC, 1982, ACS Mono. 177

Figure 1



Introduction - cont'd

Editing is done with menus and **editors**. Editors activate if their targets are present. The area where the drawing is displayed is referred to as the **Drawing**. Up, down, left and right movement is done with the arrow, Tab and Page Up and Page Down keys.

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

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.

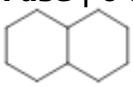
Click **Tutorial** for to learn how to draw with **ChemPen3D**

Creating a 2D Drawing with ChemPen3D -

Drawing with ChemPen3D is illustrated with the following example tutorial. Most of the drawing is done with menus and mouse clicks.

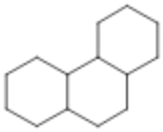
Step 1 - Add a cyclohexane ring From the main menu select **Ring, Add, 6** then click near the left side of the Drawing.

Step 2 - Fuse a second cylclohexane to the right side bond of the first. Select **Ring | Fuse | 6** and click to the right of the rightmost bond.

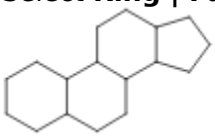


Next Step

Drawing - Step 3 - Fuse a cyclohexane to the upper rightmost bond
Click near the upper rightmost bond.



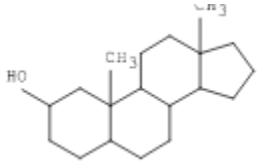
Drawing - Step 4 - Fuse a cyclopentyl ring to rightmost bond
Select **Ring | Fuse | 5** and click the left most bond bond.



Next Step **Previous Step**

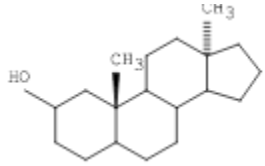
Step 5 -Branch two methyls and an OH from the previous structure as shown

1. Select **branch | CH3** and click near the two top methines
2. Select **branch | OH** an click near atom the upper leftmost methylene
3. Click **Reset** to stop branching.



Drawing Step - Modify the Methyl bonds

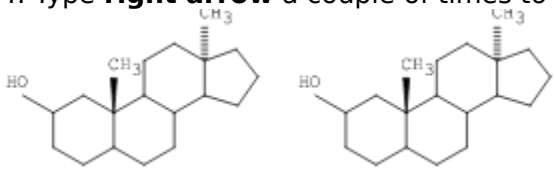
1. Hold **Shift** and click the right mouse button near the right methyl. The **Bond Editor** activates
2. Click the cross hatch symbol to change the bond to an *in plane*bond.
3. Right Click near the left methyl bond and change it to an *out plane*bond.
4. Click the **OK** button.



Next Step **Previous Step**

Step 7 - Clone the Group

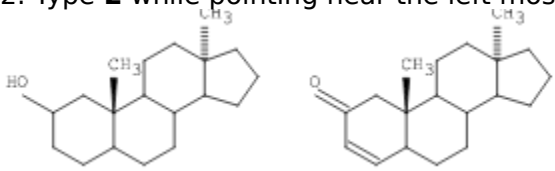
1. Drag the mouse from above left to below right of the group activating the **Group Editor**
2. Click the **Clone** button item.
3. Right button click near the new molecule to select it.
4. Type **right arrow** a couple of times to move the new structure right.



Drawing - Step 8

Create a carbonyl and a double bond

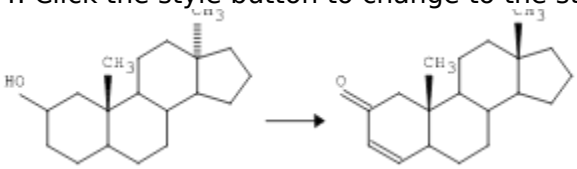
1. With the mouse pointer near the right structure's OH and type **2** carbonyl.
2. Type **2** while pointing near the left most lowest bond.



Next Step **Previous Step**

Step 9 - Add and modify an arrow

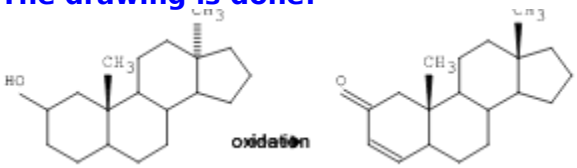
1. Select **Symbol** to activate the **Symbol Palette**
2. Select the single arrow and click between the structures to place it.
3. Click near the head or tail of the arrow. The symbol editor is activated.
4. Click the style button to change to the style below. Click the **OK** button.



Step 10 - Add a text label

1. Select **Symbol** from the main menu.
2. Select **Text** from the symbol palette and click below the arrow.
3. The text editor activates.. In the editor type the word *oxidation*
4. Hit **Enter** or the **OK** button.

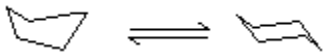
The drawing is done!



Previous Step **Table of Contents**

3D Structure Basics

Introduction to 3D Structures



While chemists draw chemical reactions as two dimensional images, molecules actually occupy three dimensional space. The atoms in a molecule are distributed in space in ways that minimize the energy of the molecule. In general molecules have more than one minimum energy 3D geometry. Examples are the boat/twist and chair structures of cyclohexane shown in the figure.

3D Energy and Geometry

The atoms in a molecule assume a 3D geometry that minimizes the molecule's total energy. The internal energy is the net sum of energy released on bond formation plus the strain energy plus the thermal kinetic energy of the atoms. If other molecules are present, the total energy is composed of the internal energy plus the energy due to interacting with neighboring molecules.

Bond lengths, bond angles, torsion angles, dihedral angles and non bonded interatomic interactions all have minimum energy values. When a molecule is strained its these values differ from their minima.

Strictly speaking , Quantum chemistry is used to calculate molecular energy and geometry. However, even today, Quantum chemistry overwhelms most PCs for all but the smallest molecules. Over the last 30 years various empirical method have been developed that do a good job of predicting molecular geometry and energy. One **the DREIDING generic force field** is used herein. DREIDING approximates molecular internal energy with sums of harmonic terms for bond lengths, bond angles, torsion and dihedral angles.

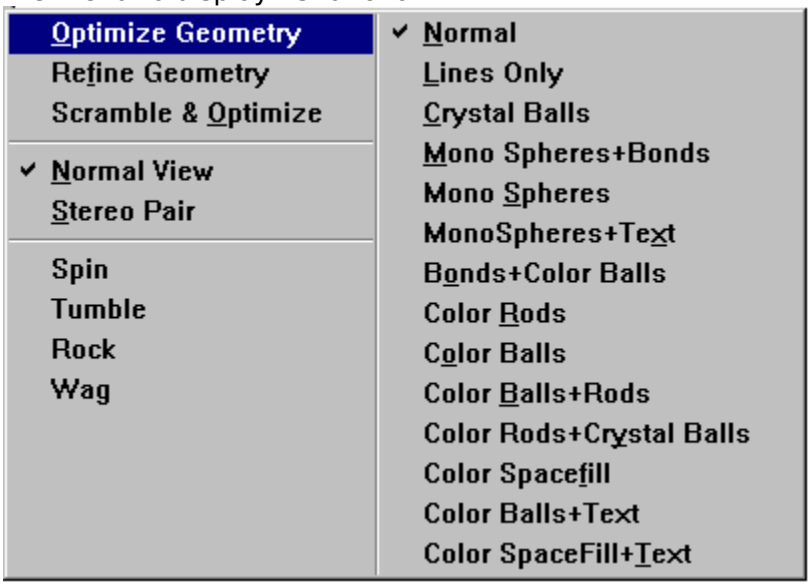
Interatomic Forces

The **DREIDING** force field includes interatomic energy terms for non bonded atoms that are not in angles torsions or dihedral coordinates. **ChemPen3D** uses the Lennard Jones potential for uncharged pairs and a simple coulomb potential for charged pairs.

DREIDING also uses a CHARMM like hydrogen bonding potential. Because non-bonded interactions are included the interaction between pairs or groups of molecules can be investigated.

The 3D Functions

From **3D Function Menu** you can optimize the molecular geometry change the 3D display, and perform some simple animation. Click on each section of the menu to display its function.



Optimizing 3D Geometry

The search for a minimum energy molecular geometry is 3D geometry optimization. In general, a given molecule will have more than one minimum energy geometry. **ChemPen3D** iteratively moves atoms to lower energy positions until the **internal energy** of the molecule has been minimized.

Optimizing Group Geometries-A group selected by the group editor can be individually optimized. This feature is used to optimize the geometries of reaction components. With the group of atoms selected, click on the appropriate 3D optimization function from the **3D Functions** menu.

Modifying 3D Geometries-A molecule can be forced into different minimum energy geometries. For example to the cyclohexane boat can be forced into the chair conformation. Use an editor to alter the molecule until it is close to the desired geometry. Then apply **Refine Geometry**

3D Drawing Tips

Draw in Normal View... While drawing can be done in any 3D view it's best to use normal. It's easier to target atoms or bonds with a mouse pointer for branching, fusing or joining of groups.

Save Your 2D Drawing First ... If you have a 2D structure you will be converting to 3D save it first under a different name and/or extension.

Use 3D Draw Mode ...3D Draw mode simplifies some drawing tasks. Rings are automatically puckered, Joined rings rotate to an orientation close to their minimum energy geometry. Drawing with 3D mode turned on can provide a visually satisfactory drawing that need not be geometry optimized. *However, for energy calculations, geometry optimization should be performed.*

Build your molecule piecemeal. For large complex molecules it can help to build your molecule piecemeal. For example to build a substituted cyclohexane, add and optimize the cyclohexane first. Then branch the groups. **ChemPen3D** takes advantage of the 3D geometry when adding a branched or fused structure.

Add Protons Last ... usually... The DREIDING works best with molecules with implicit protons. Hs should usually be added last. The **Add Protons** menu command portents a molecule, placing the protons at their correct positions in space.

Normal View/Stereo Pair

Stereo Pair view displays two views of the same drawing with slightly different parallaxes. With the proper viewer or crossed eyes you can combine these to give an apparent 3D image.

Optimize Geometry

Activates optimization routine. When launched from the main menu optimizes all atoms. When launched from the group editor menu optimizes the selected set of atoms.

Scramble and Optimize

Optimizes drawing or structure after displacing atoms by approximately one C-C bond length in random directions. This can be useful if you are trying to find other minimum energy structures.

Anneal Geometry

Annealing is repeated randomization and geometry optimization of a molecule. Annealing is most useful when a molecule is slow converging on an energy minimum.

Refine Geometry

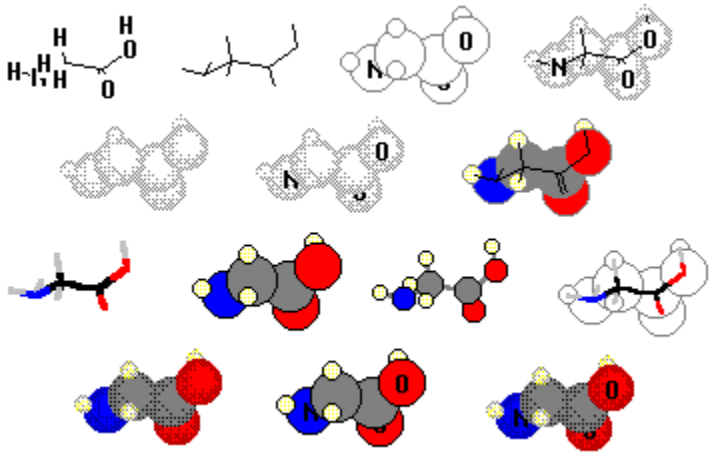
Refine geometry optimizes the drawing or selected structure after making small random perturbations to each atom. Use refine geometry if you want to nudge a molecule into an alternative geometry. For example a cyclohexane chair can be nudged into a boat if you move the an atom and invoke Refine Geometry.

Spin, Tumble, Rock, Wag

A dynamic view of a molecule can be had by one of four animation methods. **Spin** rotates the molecule around the up down(y) axis. **Tumble** rotates the molecule around its left right(x) axis. **Wag** oscillates the molecule around the y axis. **Rock** oscillates the molecule about the x axis.

3D Views

The right column of the **3D Functions** menu selects the various possible the 14 various graphic displays of the structure. The **Normal** view is the default. When a view is selected it is checked. The various views of glycine appear below in menu order.

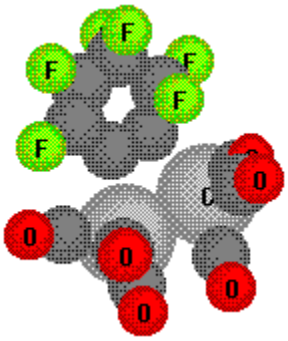


Normal and Stereo Pair Views

By default ChemPen3D displays a single structure. Select Stereo pair if you want to display two images that appear 3D when viewed via the 'cross eye' method of view.

Creating a 3D Structure

The techniques for creating a 3D drawing build on those for creating 2D drawings. Thus, you should complete the **2D Drawing Tutorial** before doing this tutorial. To illustrate, the following perfluorocyclohexa-1-3-diene tetracarbonyl complex of cobalt* will be created.



Select **3D Drawing Tutorial** to learn how to build a 3D structure.

* R. L. Hunt and G. Wilkinson, Inorg. Chem., **4**, 1270(1965),

Overview

Creating a 3D structure starts with the creation of a 2D structure. An additional optimization step converts a structure from 2D to 3D. There are a variety of 3D views that can be accessed via the **3D Functions** menu

Step 1

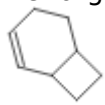
Add a cyclopropane ring by selecting **Ring | Add | 4** and clicking the drawing.

Step 2

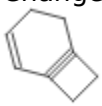
Fuse a six membered ring to the upper left bond by selecting **Ring | Fuse | 6**

Next steps

Steps 3
Change leftmost bond to double by pressing 2 with the mouse pointer over the target bond.

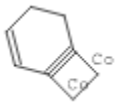


Step 4
Change fusing bond to triple by typing 3 while the mouse pointer is over that bond.



Next steps

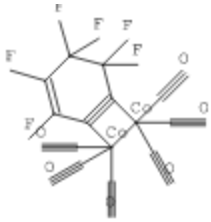
Steps 5
Select the leftmost atom by clicking near it with the right mouse button.
Click **CO**(cobalt) on the periodic table to change the atom to cobalt. Repeat the conversion for its lower left neighbor atom.



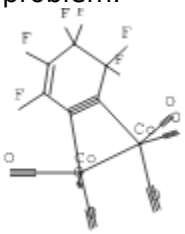
Step 6
Branch fluorine atoms from each carbon atom by selecting **branch | F** from the main menu then repeatedly clicking near each target atom

Next

Step 7
From each cobalt branch three carbonyls by selecting **branch|CO**

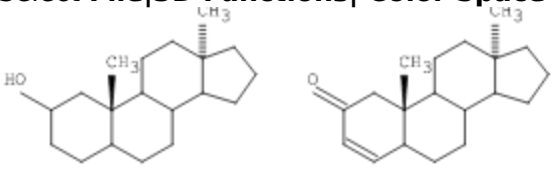


Step 8
Optimize the three dimensional structure by selecting **File|3D Functions | Optimize Structure**. For this structure optimization took about less than a minute on a 75Mhz pentium. Typically, the structure becomes highly distorted during optimization. This is not a problem.

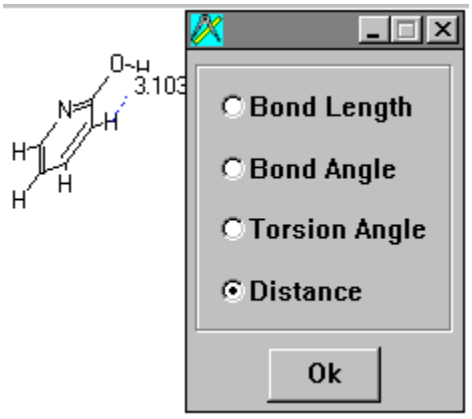


Finally

Final Step
Select **File|3D Functions| Color Space Fill** to give...



The Measurement Tool



Four geometric properties, bond length, bond angle, torsion or dihedral angle and interatomic distance are measured with the measurement tool.

To display bond length, bond angle or torsion angle select the appropriate radio button and click near the target internal coordinate. The value is displayed near the target.

To display interatomic distance click near the *anchor* atom. Click near any other atom to display the interatomic distance in angstroms. To select another anchor, click near the current anchor to clear it . Then click near the new anchor and repeat the above procedure.

Menu Commands

All drawing is done from the **Main Menu** shown below.

File	**Reset**
Alkane	**Ring**
Atoms	**Symbol**
Branch	**Symbol|Text**
Benzene	**Symbol | Formula**
Font	**Undo/Redo**
Link	

Using the Keyboard

The keyboard can be used to navigate **ChemPen3D**. The following key commands move the drawing without affecting the scroller.

Arrow keys move the drawing up, down, left and right by **jump** units.

Shift | Arrow moves the drawing or selected group by 32 units.

An atom can be changed to one of several non-metal elements with a single key stroke . Point to the atom and type one of the following:

H-hydrogen, **C**-carbon, **N**-nitrogen, **O**-oxygen, **B**-boron, **F**-fluorine, **X** - chlorine, **Y** - bromine, **I** - iodine , **Q** - silicon, **P** - phosphorous, **S** - sulfur, **Z**- selenium

A bond type can be changed by a single keystroke. Point to a bond and type one of the following keys.

1-single bond, **2-**double bond, **3-**triple bond, **4-**resonance or transition double bond, **5** transition state bond, **6** triple resonance, **A-**toggles a bond between aromatic and non aromatic *
K- deletes a bond, **L-**links the two closest atoms with a new bond
+ , = (plus) increases the charge of the closest atom by 1,
- (minus) decreases the charge of the closest atom by 1.

Also see: **Entering and Editing Text**

Overview of Editing

ChemPen3D 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.

Atom Editor

Bond Editor

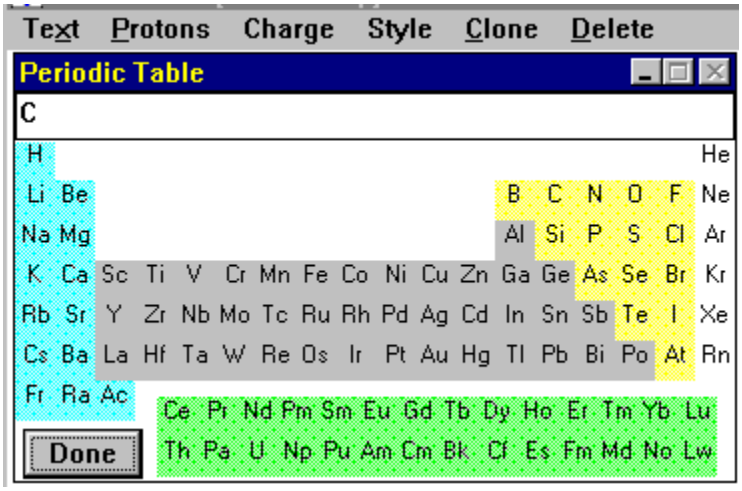
Group or Ring

Symbol

Text Editor

Also see **Introduction**

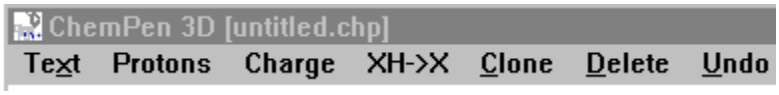
Editing Atoms



Editing atoms is done with the atom editor and the **Atom Editor Menu** .To activate the **Atom Editor** below right mouse button click near the target atom. Use the Atom Editor's buttons, menus and text editor to change the currently selected atom.

Also see Editing ,**Menu Commands**

Atom Editor and Atom Editor Menu Commands



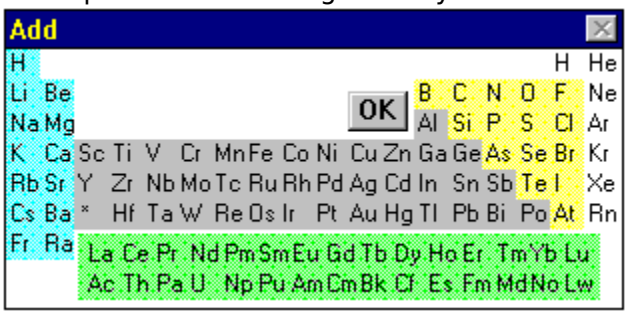
Text Window - edit text in the text window.

Menu commands

Text | L/R shifts symbol between left and right.
Text | Reflect reverses order of characters.
Text | Font select to change symbol font
Protons +H, -H add or an H. **+H(+), -H(+)** add or subtract a proton.
Charge increase or decrease an atom's charge by one.
X->XH toggle non-metal symbol between **A**, **AHn** and none
Clone generates a clone of the selected atom.
Delete deletes selected atom and deletes any attached bonds.
Undo reverses editing.

Add/Branch Atom

Launches periodic table. From it select an atom to add to the drawing. Click the spot on the drawing where you want to add or branch the atom.



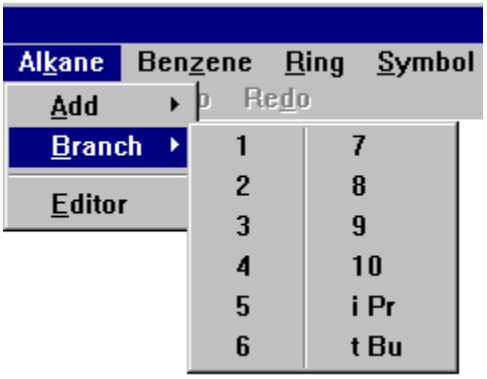
Also see: **Menu Commands**

Branch

Branch a single bond, a hydrogen, a halogen atom, or one of several common functional groups from an existing atom.

bond	CH2OH	NH2	OH	SH
CH3	CHO	NHCH3	=O	=S
H	COCH3	NHCOCH3	OCH3	SCH3
F	CONH2	NCO	OCOCH3	SCOCH3
Cl	COOH	NO2	OCOOH	SO3H
Br	=CH2	=NH	PH2	SO2NH2
I	CH=CH2	=NOH	OP(OH)2	SO2
CN	CH=C=CH2	=N=O	PO(OH)2	SO2CH3
	C%CH	N%CH	OPO(OH)2	
		NO		

Alkane Menu

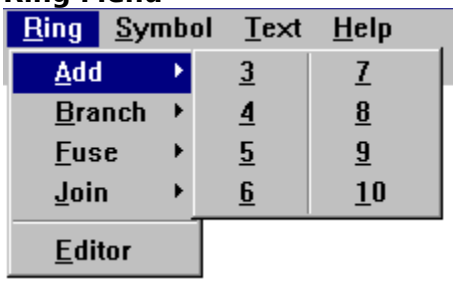


Alkanes are **added** to the drawing or **branched** from existing atoms by selecting them from the alkane menu. T-butyl can be added. T-Butyl and i-propyl can also be branched.

Benzene Menu

Select the appropriate menu item to **add** benzene to a drawing, **branch** benzene from an atom or **fuse** benzene to a bond.

Ring Menu



Select the appropriate menu item to **add** a ring to a drawing, **branch** a ring from an atom, **join** a ring to an atom or **fuse** a ring to a bond.

Labels and Formulas

ChemPen3D uses two label types; texts and formulas. Text is entered and edited with the **Text Editor** below.

To enter text, select label from the **Symbol** palette and click the spot where you want to add text. To edit and existing click near the label with the right button. Use the same method to create and edit a formula. When the text editor is active a text can be dragged by the mouse.

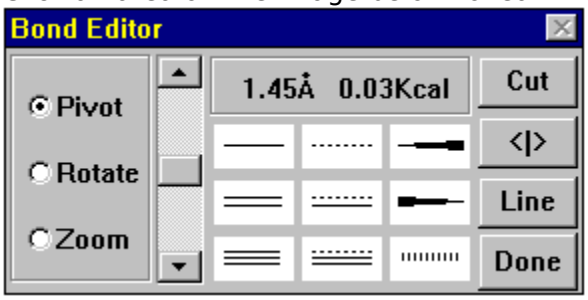
Also see **Editing**

Reset
Turns off drawing command repetition. If a drawing command, for example **Branch | COOH** is invoked, repeated clicking on the drawing 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.

Editing Bonds

The bond editor is used to edit bonds. Click the right mouse button while holding **shift** and pointing near the target bond to activate the bond editor. Click an area on the image below to learn its function.



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

Bond Editor Data Box
Displays the bond length in angstroms and bond strain energy, as computed by the DREIDING force field in kcal. This only has relevance for 3D structures generated by ChemPen3D.

Bond Type
To change to a bond type select its image.

Bond Editor Button Functions

Cut deletes bond and updates atoms valences.

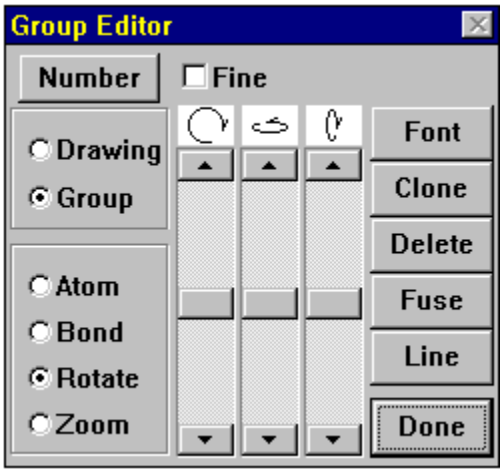
<|>toggles multiple bonds between left, right and center.

Line toggles bond thickness between 0,1,2,3.

Bond Editor Slider

The bond editor slider pivots, rotates or zooms the selected bond depending on the setting of the radio buttons. Select **Pivot** to pivot the bond around one of its atom. Click near the pivot atom to select it. **Rotate** rotates bond within the plane and around the bond's center. **Zoom** increases or decreases the length of the bond around its center.

Group Editor



Groups are edited with the group editor and its menu. To activate, hold **Ctrl** and click the right mouse button while pointing near the target group. Alternately drag the mouse from left and above the group to right and below. Click the area on the image at left to learn its function.
Also see **Editing** ,**Menu Commands**

Group Editor Buttons

Font - change group font

Clone -duplicate group.

Delete - delete group

Fuse - fuse selected atoms and bonds into new group.

Line - toggle line thickness between 0,1,2,3.

Number numbers atoms in group starting at 1 if the **Group** radio button is selected or at the highest Drawing number if **Drawing** is selected..

Group Slider Functions

The function of the slider is determined by the selected radio button.

Fine check box sets the rotation range to ±30° from ±180°. If the Zoom function is selected the zoom range is set to ±10% from ±50%.

Tilt, and **Turn** rotate the group around vertical or horizontal axes

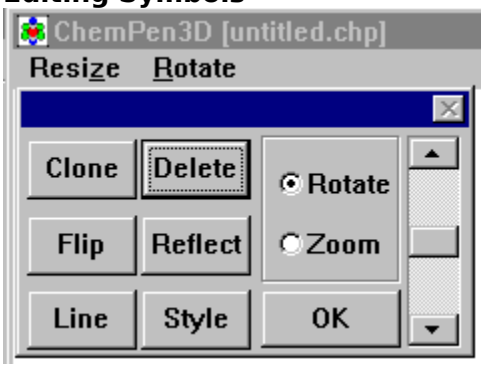
Rotate rotates group within drawing plane.

Atom selects pivoting around an atom. Click near the pivot atom to select it. Pivot the group around the atom by moving the appropriate slider.

Bond selects pivoting around a group. Click the pivot bond to select it. Pivot the group around the bond by moving the **Pivot** slider.

Zoom continuously enlarges or shrinks the selected group.

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. Click each part of the illustration in this figure to learn its function.

Also see **Editing**

Symbol Editor Menus and Buttons

Rotate **90°,-90°,+45°,-45°** rotate some symbols by the angle shown.

Zoom **+50%, -50%** zooms the symbol by the amount shown

Reflect and **Flip** reverse some symbols up/down or left right.

Line changes the line thickness

Style affect depends on the symbol

Clone creates a duplicate of the selected symbol

Delete deletes the selected symbol

Symbol Editor Radio Buttons
The radio buttons determine the function of the slider namely **Zoom** or **Rotate** The slider rotates or zooms the symbols depending on the setting of the radio buttons.

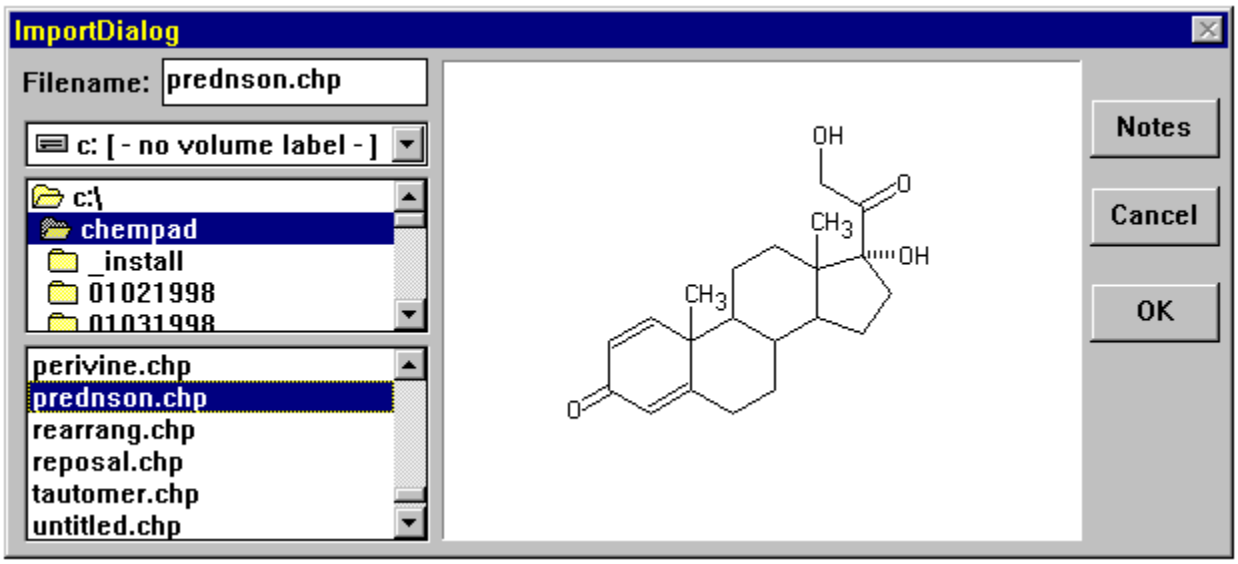
File Menu

Opening, saving and exchanging **ChemPen3D** drawings is done, from the **File Menu.** The relevent parts of the filemenu appear to the left. Click on each menu item to learn its function.

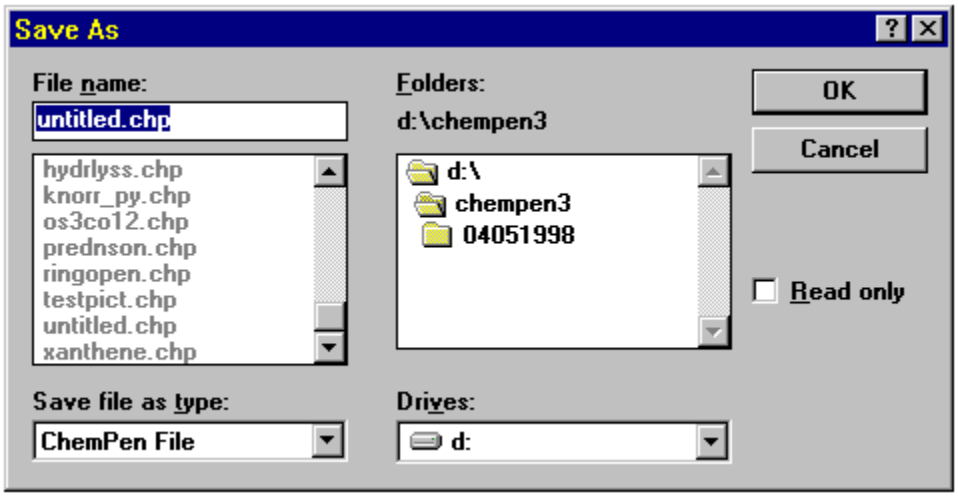
Also see **Menu Commands**

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

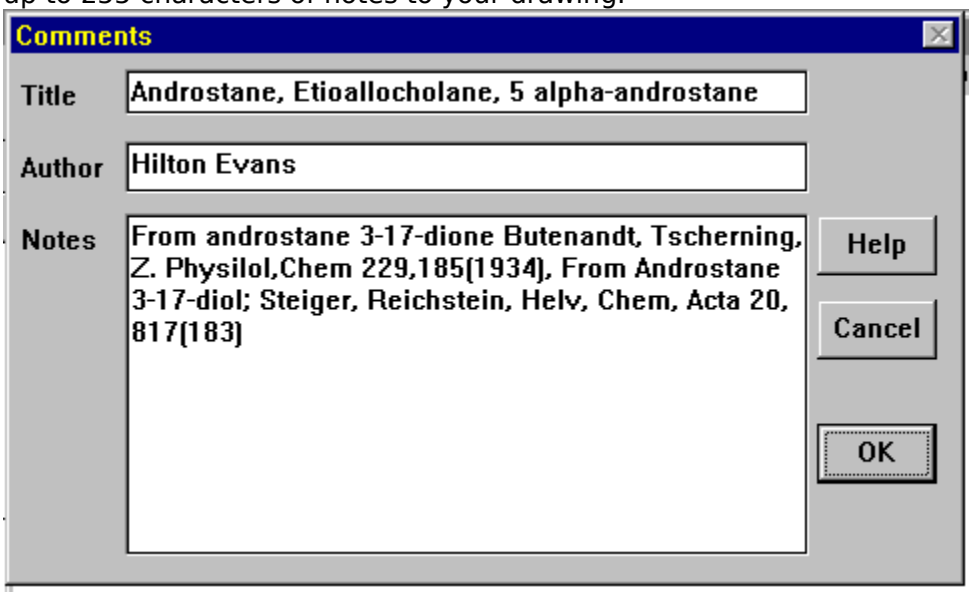
File Open executes the **file open dialog** below. The **Preview** window lets you see a scaled down view of the selected file. The **information** button will display any information entered by the creator. Click each part of the figure to learn its function. If you click the **OK** button the previewed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



File | Save , File | SaveAs
executes 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 demonstration version of ChemPen3D**.



File Comments ... executes the **Information** dialog. Add a title, author and up to 255 characters of notes to your drawing.



File | CopyToClipboard

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

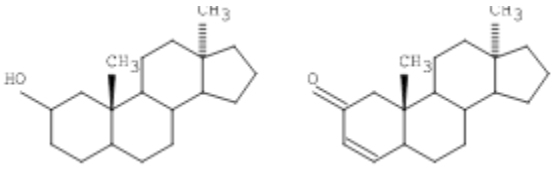
Bit maps are raster representations of pictures. **ChemPen3D** copies its drawings to the clipboard in metafile or bit map format. Compared to metafiles, bitmaps draw themselves very fast. However bitmaps zoom poorly and should not be used where they must be resized.

Metafiles

Metafiles are sets of instructions that represent a drawing. **ChemPen3D** copies drawings to the clipboard in metafile or bit map format. Metafiles can be resized continuously but compared to bit maps draw themselves slowly.

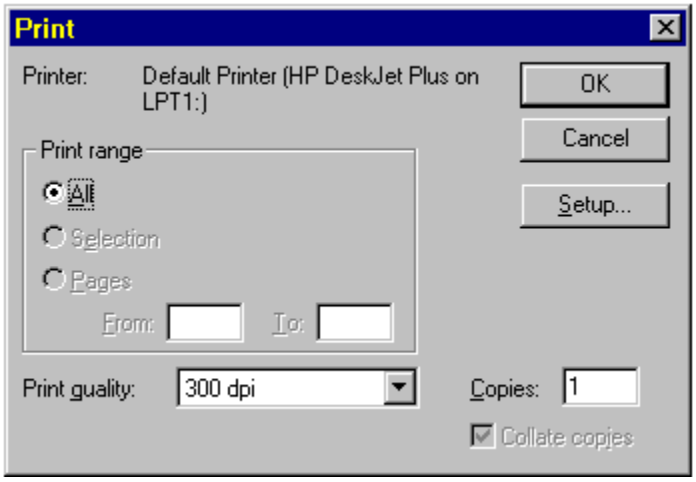
File | Import

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.

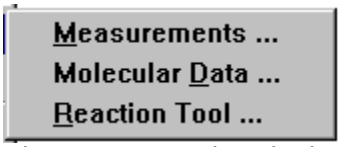


File | Print

Opens the print dialog from which you can print your drawing. The printer can also be setup from this dialog assuming you have installed drivers appropriate to your printer. You can also copy and paste a drawing into a graphic word processor, such as Winwrite® or WordPad ® and printed.



Chemistry Menu



ChemPen3D's chemical property predictions and calculations are accessed from the **Chemistry Menu.** Click on each menu item to display its function

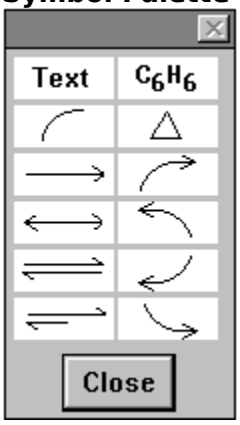
File Defaults

Use **Default Settings** to set the default values for **line width, jump size,** and **bond length.** The information is saved in file named **chempen3.cfg** or **chempen3d98.cfg** . **Chempen3.cfg** / **chempen3d98.cfg** is saved in the Windows directory. The drawing is initialized with the **chempen3.cfg** / **chempen3d98.cfg** data. If **chempen3.cfg** / **chempen3d98.cfg** does not exist it is created upon starting **ChemPen**. with a set of default values.

*jump size is the distance a drawing or selected group is moved when an arrow key is pressed.

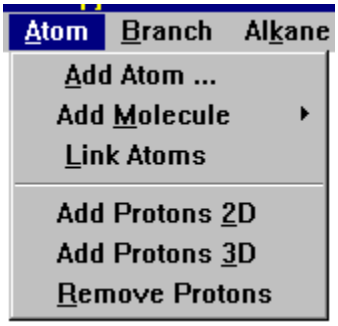
File Exit
Shuts down the application. If a drawing exists you are prompted to save it.

Symbol Palette



Symbols such as, , are added to a drawing using the symbol menu. Examples of symbols are arcs, arrows and the triangle. Symbols can be edited with the Symbol Editor. As **ChemPen3D** is developed other symbols will be added.

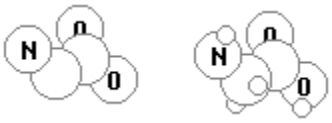
Atom



From the **Atom Menu** you add atoms, link(form single bonds) atoms, add protons to or remove protons from a molecule or add on of several small common molecules. Click on the menu below to learn its function.

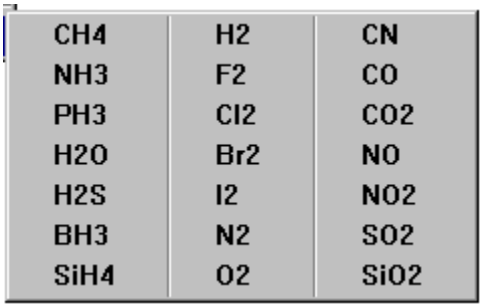
Add Hs/Remove Hs

Use **Add Hs 2D** if you want protonate a 2D drawing. You can also protonate a group or individual atom by selecting it. Use **Add Hs 3D** to protonate a drawing distributed in 3D. To remove protons select **Remove Hs**. Molecules with and without explicit protons appear below.



Add Molecule

Add one of several common small 3D molecules from this menu.



Link Atoms

Connects two atoms with a single bond. Select this menu item then click near each atom to be bonded. An error occurs if you click near the same atom twice.

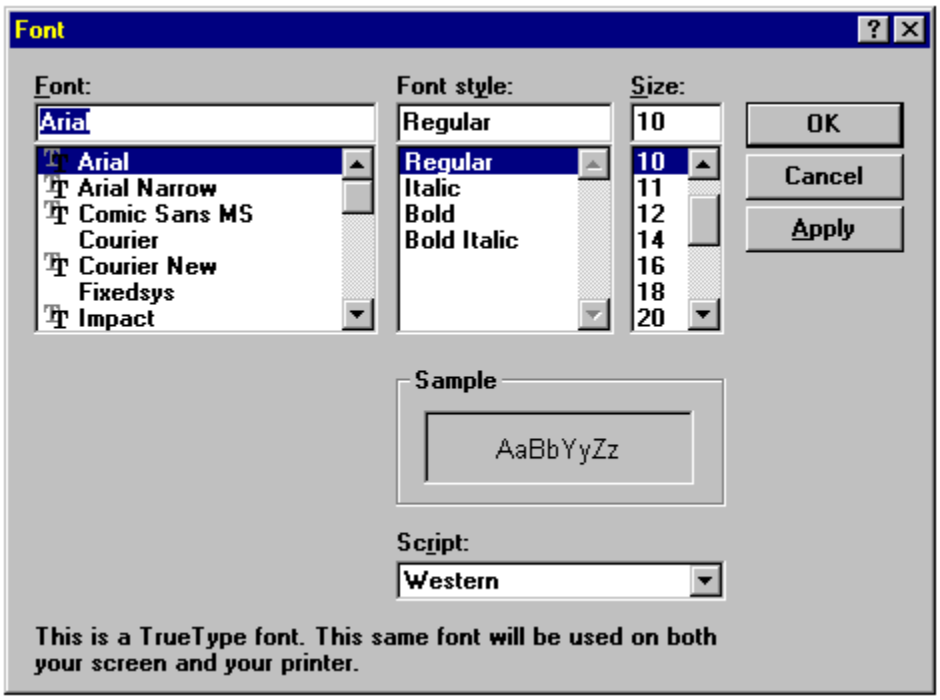
Ring

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.

Font

Launches the **font dialog** allowing the user to change the *drawing's* font.

Font Dialog


Font
Font:
Aria
Arial
Arial Narrow
Comic Sans MS
Courier
Courier New
Fixedsys
Impact
Font style:
Regular
Regular
Italic
Bold
Bold Italic
Size:
10
10
11
12
14
16
18
20
OK
Cancel
Apply
Sample
AaBbYyZz
Script:
Western
This is a TrueType font. This same font will be used on both your screen and your printer.

Link

Found under the **Atoms** menu, **Link** is used to form a new bond between two existing atoms select link then click near each of the two atoms. Use **RESET** to stop linking. You can also link to close neighbor atoms by typing **L** with the mouse pointer between them.

Using the Mouse

ChemPen3D makes extensive use of the mouse in drawing and editing. Additional functions are provided by combining the left and right mouse buttons with the shift and control keys.

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

The **Shift|right mouse button** - selects the nearest **bond** and activates the **bond editor**

The **Ctrl |right mouse button** - selects the nearest **group** and activates the **Group Editor**.

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

Also see **Editing**

Molecular Properties

Molecular properties are displayed in the Molecular Properties Dialog. A molecule should be geometry optimized before its properties are diaplayed.

{moledat3.shg}

Moments of Inertia

ChemPen3D can report the principal moments of inertia, in amu x Å, for a 3D optimized molecule. To display the principal moments of inertia select **File | Chemistry | Moments of Inertia**

Strain Energy

Strain energy results when internal coordinates deviate from their minimum energy values. The Bond Editor displays the strain energy of an individual bond.

Internal Energy

The internal energy of a 3D geometry optimized molecule can be estimated. The internal energy is the sum of the bond energies plus the net steric strain energy plus the kinetic energy of the molecule.

Dipole Moment

Given an optimized 3D structure, **ChemPen3D** can estimate the dipole moment of a molecule. Select **File | Chemistry | Dipole Moment** and an estimate of the dipole moment is displayed in a dialog box.

Molecular Data

ChemPen3D calculates a molecules formula weight, chemical formula and percent chemical composition. To display a molecule's data select **File | Chemistry | Molecular Data**

Chemical Reactions

Introduction to Chemical Reactions

With **ChemPen3D** you can analyze reaction energetics. A byproduct of 3D geometry optimization is the internal energy. Herein the internal energy is the energy released on bond formation + total strain energy + thermal kinetic energy. Strain energy results when bond lengths or angles and torsion or dihedral angles deviate from their minimum energy values.

ChemPen3D does all reaction calculations assuming gas phase. Gibbs free energy, enthalpy, entropy and the equilibrium constant are calculated and displayed by the reaction tool. The reaction tool is also used to balance the reaction and adjust temperature and pressure.

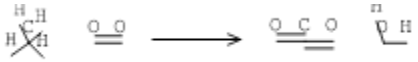
Beginning **Building A Reaction**

Building a Reaction

Building a reaction is simple. Products and reactants are placed to the left and right of an arrow. Arc arrows should not be used. Other symbols, formulas and labels, are ignored. Only the first arrow added to the drawing is recognized.

Fuse each reactant!

Each reactant or product must be individually 3D geometry *optimized and fused*. It's a good idea to select and fuse each reactant or product after building a reaction. The reaction for the combustion of methane is shown below.



Beginning **Balancing Reactions**

Balancing Reactions

A reaction is balanced with the Reaction Tool With a reaction built and groups optimized, select **File | Chemistry | Reaction Tool** to launch the reaction tool.

Adjust the moles of each substance using the scrollers in the **Substance Info.** box until the **Mass Balance** message box reads BALANCED. Balance is also when the elemental molar balances in the lower window all vanish. Balancing takes account of the *implicit protons* in certain non metal atoms.

Beginning **Analyzing Reaction Energetics**

Analyzing Reaction Energetics

The energetics of a reaction can be analyzed using the **Reaction Tool** **ChemPen3D** uses its modified DREIDING force field to predict a molecule's heat of formation. ChemPen3D treats a molecule as forming from individual atoms; each with a zero reference energy. Select the **Report** button to copy a summary of the reaction's energetics to the clipboard.

Beginning **Protons in Reactions**

Protons In Reactions

Protons can be implicit  or explicit

 . For reaction energy calculations **ChemPen3D** only takes account of the bond energies of explicit **X-H** bonds.

1. If proton bonds are broken in a reaction, explicit protons should be used.
2. You don't necessarily have to protonate every atom when protons are used. You need only protonate the atoms that are actually involved in X-H bond breakage.

Beginning **Things to Remember**

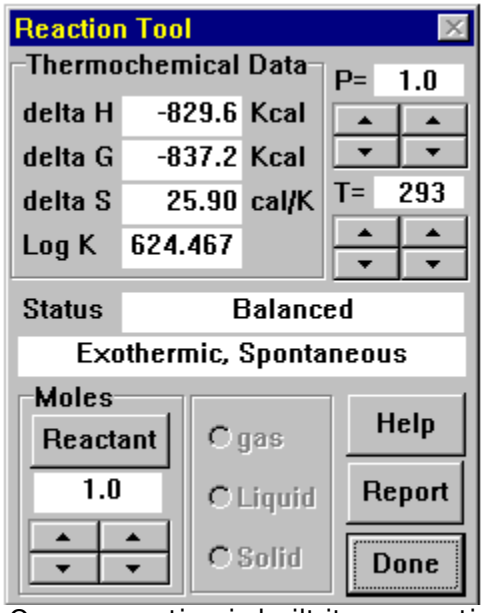
Things to Remember

1. The reaction tool only works with one reaction per drawing.
2. A reaction is a set of molecules left and right of an arrow.
3. Only the first arrow is recognized by a reaction.
4. Arc arrows are not recognized
5. Each molecule must be individually 3D optimized, and fused.
6. In ChemPen3D reactions are treated as gas phase*.
7. Add explicit protons only when needed.

***PChemPen3D,** a more sophisticated version of ChemPen3D will lets you treat reactions in solution.

Chemical Reactions

ChemPen3D Reaction Tool



Once a reaction is built its energetics can be analyzed using the Reaction Tool. To activate the reaction dialog, select **File | Chemistry | Reaction Tool.** Click on the graphic below to determine each reaction tool function.

Note: The reaction tool switches the drawing to normal view

A Balanced Reaction

The balanced combustion reaction of methane is shown. The coefficient of each reactant or product appears below the reaction.

Substance Information

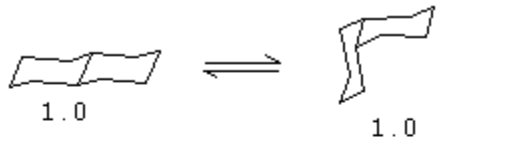
The **Reactant** button tabs between reactants. The selected reactant is highlighted in red.

The number of moles of the selected substance is adjusted by the scrollers in this box. Moles can be adjusted to 0.1 mole.

The state buttons inactive in ChemPen3D are a feature of the more advanced PChemPen3D due the second quarter of 1998.

Reaction Summary

An image of the reaction and a summary of its thermodynamic quantities is copied to the clipboard by the **Report** button. The report can be pasted into a word processor. A copy of the report simultaneously appears on the screen. An example appears below.



trans-decalin cis-decalin

Summary
P = 1.0 T = 293K
deltaG = 1.5 Kcal
deltaH = 1.5 Kcal
deltaS = 0.00 cal/K
lcgK = -1.143

Pressure and Temperature

The Pressure and Temperature are set, respectively using the **P(atm)** and **T(K)** scrollers.

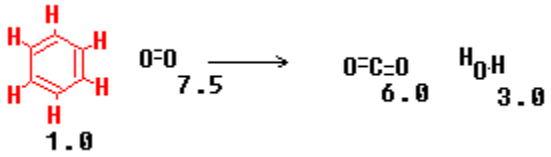
Reactant Button

The reactant button tabs between reactants and products.

Upon selection the compound is highlighted.

Mass Balance

The mass balance message box aids you in balancing your reaction. The UNBALANCED message changes to BALANCED when the reaction is balanced.The second lower box shows the difference in moles between reactant and product atom counts. The mole difference for each element reads 0.0 when that element is balance. The coefficient of each compound appears below the compound. A balanced reaction appears below. The reaction tool is not shown.



Thermodynamic Functions

The enthalpy, free energy, entropy and logK appear in the left column of the Thermochemical Data box. In ChemPen3D all calculations are done in the gas phase. In the more advanced PChemPen3D (available Q2 1998) estimations can be made on reactions in solution

About PChemPen3D

Available the Second Quarter of 1998, PChemPen3D is Physical ChemPen3D. PChemPen3D extends the functionality of ChemPen3D. PChemPen3D adds solution property prediction, reactions in solution and reaction rate constant prediction. News about ChemPen3D and PChemPen3D.

http://home.ici.net/~hfevans/chempen3.htm

Registering/Ordering ChemPen3D

Customers ordering **ChemPen, ChemPen98, ChemPen3D** or **ChemPen3D98** over the internet receive an unlock code by e-mail. Those ordering disks, will receive a disk and booklet in about 2 weeks in addition to receiving an unlock code.

1. ChemPen3D over secure Internet form via **Northstar Solutions, Inc**.
Point your web browser to **http://www.nstarsolutions.com/1078.htm**

2. PHONE 800 699-6395 or 785 539-3731
(am - 7 pm, CST, Monday - Friday)

3. MAIL Orders

4. FAX ORDERS

5. E-MAIL Orders:

Compuserve: starmail

America Online: starmail

Internet: Starmail@compuserve.com

6. Compuserve members: GO SWREG:

ChemPen ID: 11961

ChemPen3D ID: 16810

7. Check or Money Order Form

ChemPen/ChemPen3D Credit Card Order Form

Name:_____

Address:_____

Town/City:_____State: _____Zip Code_____

Email Address_____

Phone Day:_____Phone Evening_____

Operating System _____ Windows 95/Windows NT _____Windows 3.1

ChemPen (2822) Copies: _____X $39 + $0.00 E-Mail S&H Total_____

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Mail this form to :

Hilton Evans
232 Canton Street 312
Randolph MA 02368

Contact **hfevans@compuserve.com** to verify address.

Customer Support

Customer Support for **ChemPen3D** is available to registered users **internet mail** or **Compuserve Mail**. If you have a question, want to report a bug or have a problem with **ChemPen3D** write to the following. For registered copies be sure to include your registration number in any correspondence.

Compuserve: 102303.2120

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