

# ACD/ChemSketch

Version 11.0 for Microsoft Windows

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## Tutorial

### *Drawing Chemical Structures and Graphical Images*

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## Before You Begin

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Thank you for purchasing ACD/ChemSketch. We have endeavored to produce the easiest to use, most powerful program for drawing chemical structures, reactions, schematic diagrams, and designing other chemistry-related reports and presentations.

### *Freeware Version*

From April 1999 onward, Advanced Chemistry Development, Inc., (ACD/Labs) has been making ACD/ChemSketch available as freeware, through the "Free Stuff" link at our Web site.

**Important** ACD/ChemSketch freeware should be installed in its own separate folder. This folder can contain other ACD/Labs freeware concurrently available but it **should not contain any purchased ACD/Labs software.**

All of the limitations on Freeware and also the Frequently Asked Questions (FAQs) can be found on our Web site at [http://www.acdlabs.com/products/chem\\_dsn\\_lab/chemsketch/tech.html](http://www.acdlabs.com/products/chem_dsn_lab/chemsketch/tech.html).

**Note** Although ACD/ChemSketch freeware does not entitle you to technical support, we encourage you to visit the ChemSketch newsgroup at the address mentioned in the *How to Contact Us* section where you can post your questions or share tips.

### *About This Tutorial*

Completion of this tutorial should give you the tools needed to get started with ACD/ChemSketch, it is designed for either online use or to be printed and used as a "hard copy" version.

The screen shots shown throughout this tutorial have been taken with a relatively small window size.

The colors and other properties of the window elements described throughout this tutorial correspond with the default Windows Display Properties.

This tutorial is provided in electronic form, readable with Adobe Acrobat software. If you cannot locate an index topic you need please do a text string search for the relevant word or phrase, or related words.

## Advanced Understanding

This tutorial is intended to be a part of the technical documentation for ACD/Labs software. To study ACD/Labs products gradually, we recommend the following order of working through the technical documentation (the corresponding documents are located in the ACD/Labs documentation folder, \DOCS):


1. Reference manual (CHEMSK\_R.PDF) and tutorial (the current document) for ACD/ChemSketch
2. User's Guides for ACD/Dictionary (DICT.PDF) and ACD/3D Viewer (3D.PDF) that familiarizes you with features of drawing and looking up structures.

In addition, it is advisable to have knowledge of the following ACD/Labs products (the corresponding documents are located in the ACD/Labs documentation folder, \DOCS):

1. ACD/I-Lab (ILAB.PDF)—the Internet-based service that allows you to get instant access to chemical databases and property predictions programs (can be downloaded from <http://www.acdlabs.com> for free).
2. ACD/ChemBasic (CHEMBAS.PDF)—the special programming language that enables the user to customize ACD/Labs software (can be downloaded from <http://www.acdlabs.com> for free).
3. ACD/Name to Structure (NAMESTR.PDF)—generates a molecular structure for almost any chemical name. ACD/Name to Structure processes the majority of the names of general organic compounds and many natural product derivatives according to IUPAC Recommendations on Organic, Biochemical, and Inorganic Nomenclature (should be purchased in addition to ACD/ChemSketch).

## Mouse Conventions

You may perform several actions during your work with this software; the following specific words are used to describe them:

- **Point to** means move the mouse pointer  to an item.
- **Click** or left-click means point to an item, and press the left mouse button.
- **Right-click** means point to an item, and press the right mouse button.
- **Double-click** means point to an item, and quickly press the left mouse button twice.
- **Drag** means point to an item, and press and hold down the left mouse button while you move the item.
- **Select** means highlight or make an interface element active by either clicking it or dragging over it (other actions are possible if specified in documentation). If used in "select the check box", it means that the check box should be marked with a tick (as opposed to "clear the check box" when the check box should be cleared, without a mark).



## For More Information...

To see the latest in ACD/Labs software and services, please visit our Web site at

<http://www.acdlabs.com/>

Our Web site is being accessed at the rate of tens of thousands of "hits" per day. There's a reason for this: much is offered through our Web site. As of Autumn 2007, we offer free ChemSketch 11.0, an ACD/LogP Freeware Add-on for ChemSketch, a free ISIS 3D Add-in, free ChemDraw extensions, and a free 2-week demo key for "Interactive Laboratory" sessions where you can run test calculations using Java applets without purchasing software. There are TechSmith Camtasia-based movies which show the operation of many of our software packages (especially ChemSketch) available for download.

We are constantly updating the information on our Web site. The Web site will tell you at which scientific conferences you can visit the ACD/Labs booth. You can browse the Frequently Asked Questions page or drop in and "chat" on our newsgroup, which can also be reached via our web page.

If you would like to stay informed of the latest developments in chemical software at ACD/Labs, please be sure to sign up for e-mail broadcasts at our Web site page:

<http://www.acdlabs.com/feedback/mailing.html>

If you would like to participate in the ACD/Labs forums, please access:

<http://forum.acdlabs.com>

## How to Contact Us

We are accessible through our Web site, phone, fax, and regular mail, but by far the most popular way to contact us is via electronic mail. Questions on pricing, sales, availability, and general issues should be directed to:

**info@acdlabs.com**

Technical and scientific support issues should be addressed by visiting:

<http://support.acdlabs.com>

Please tell us the name of the software purchaser; the product name, version number, build number, and license ID of the product you are contacting us about (from the **Help** menu, choose **About** to find this information); as well as a description of the problem you are having. If applicable, please tell us the name of the distributor from whom you purchased the software.

## Online Updates

All PC-based ACD/Labs software contains the capability to have software updates delivered online. You will need the registration numbers of the software and an Internet connection from the same computer on which the software is installed. The updates are small fixes, for example, bringing the actual version number of a program from 11.00 to 11.01. For more information on this, please refer to the document located in the ACD/Labs documentation folder, \\DOCS\\UP\_CLNT.PDF, or contact our technical support department.

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# 1. Basics of ACD/ChemSketch

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## 1.1 Objectives

This chapter will familiarize you with

- How to start the program;
- How to set and change file associations;
- How to set default directories; and
- How to quit ChemSketch.

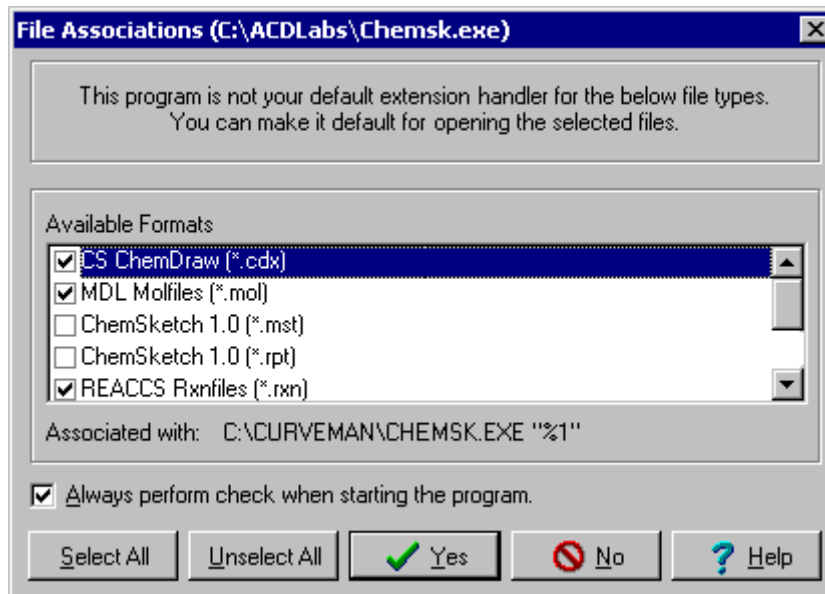
## 1.2 Starting ACD/ChemSketch

Once ACD/ChemSketch has been installed on your computer, follow these basic steps to start it:

1. Start Microsoft Windows.
2. Double-click the ChemSketch icon.  
–OR–  
From the **Start** menu, point to **ACD/Labs** and then choose the ChemSketch icon.  
–OR–  
Double-click the program file CHEMSK.EXE in the folder where you have installed all ACD/Labs software. By default, this is ACD11.  
–OR–  
If you have other ACD/Labs programs running, from the **ACD/Labs** menu, choose **ChemSketch**.
3. You should see an opening splash screen. If this is the freeware version, you will see the **ACD/Labs Products** screen. Click **OK** to close it. If you wish to suppress this dialog box for the subsequent startups, from the **Help** menu, choose **ACD/Labs Products** and clear the **Show this Screen at Startup** check box.

## 1.3 Setting File Associations

If you run ACD/ChemSketch for the first time, the **File Associations** dialog box appears:



It contains a selectable list of file extensions and file types, e.g. CS ChemDraw (\*.CDX), REACCS Rxnfiles (\*.RXN), ISIS/Sketch (\*.SKC) which you may want to open automatically with ACD/Labs software from now on. If so, click the check boxes of the file formats you want to add, and then click **Yes**.

If you do not want ACD/ChemSketch to open files with the listed extension automatically, or are not sure, leave the check boxes blank and click **No**.

Then you will see a **Tip of the Day** box, which you can close after reading.

### 1.3.1 Changing File Associations

If you have not selected all formats, the default file association can be viewed or changed at any time; from the **File** menu, choose **File Associations**.

**Note** If you choose **File Associations** under Windows NT while you are not entitled to change file associations in the system, a warning message appears. Contact your system administrator to resolve the matter.

If all formats are selected, you receive a message, "all supported file types are already associated with the current application." In this case, you can change the file associations through **Windows Explorer**.

1. Open Windows Explorer, and select a file with the extension for which you want to create the association.
2. Hold down SHIFT and right-click the file name. From the shortcut menu, choose **Open With**. Note that in some Windows operating systems (e.g., Windows XP) you do not have to press SHIFT to get **Open With** on the shortcut menu.

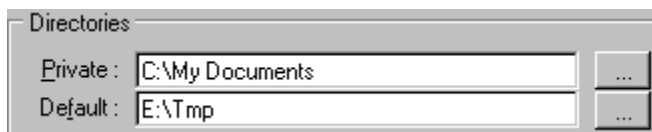
3. Set the application that should be used to open the file and select the **Always use this program** check box.
4. Click **OK** and close Windows Explorer.

## 1.4 Changing Default Directories

If you are running a single-user (stand-alone) copy of ACD/ChemSketch, the default directory settings are likely appropriate.

If you have a network copy, it is advisable to change the default directory settings in the ACD/Labs software so that the default drive for saving work-in-progress is the user's local hard drive, not the remote server. After creating local access for either limited or unlimited number of seats, then at each local installation:

1. In the ChemSketch window, from the **Options** menu, choose **Preferences**.
2. In the dialog box that appears (note that the **General** tab is active), under **Directories**, in the **Default** box, specify the directory that will be opened every time you open the **Import**, **Open**, **Save**, or **Export** dialog boxes in the ChemSketch window:



**Note** In the **Private** box, you can set the directory for recording the configuration of ACD/ChemSketch (e.g., TEMPLATE.CFG and QRSTYLES.STL files).

3. Click **OK**.

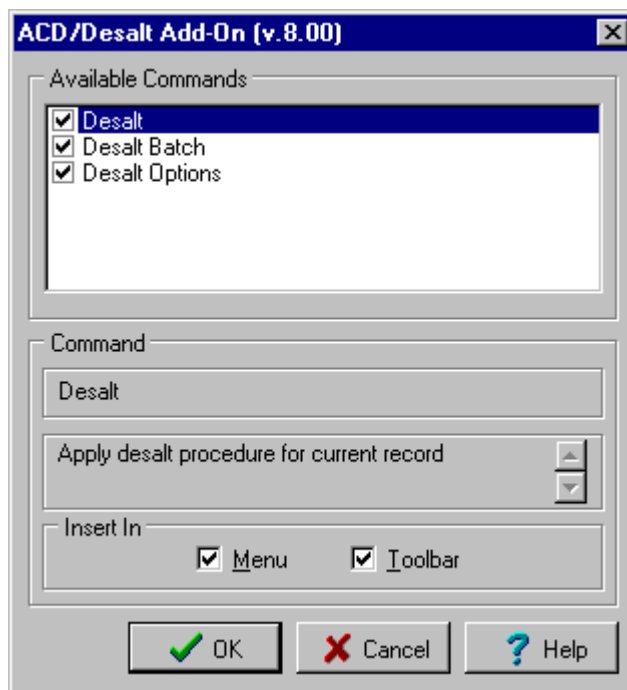
## 1.5 Installing Add-ons

Starting from version 8.0, it is possible to install add-ons—small programs (with .ADDON extension) written to extend the features of the main application. Each add-on contains a set of commands to be applied either to the current record or to the whole database (so called, *batch* commands). As soon as the add-on is installed, its commands can be placed either on the toolbar as buttons or on the main menu as commands of the **Add-on** submenu (**Database** and/or **Record** menu), or both.

To install the add-on, follow the steps below.

1. From the **Options** menu, choose **Add-on Organizer**.
2. Click **Add** and, in the **Open** dialog box that appears, find the .ADDON file. Click **Open** to add it to the list.


3. To customize some of the add-on options, select it in the list and click **Edit**:



4. In the **Available Commands** box, select the commands to be accessible from the ChemSketch interface. In the **Insert In** area, choose where the add-on commands should be added: as commands to the menu and/or as buttons to the General toolbar (if it was implemented by the add-on author). Click **OK**.
5. Click **OK** in the **Add-on Organizer** dialog box and verify whether the menus or buttons are added to the interface.

## 1.6 Quitting ChemSketch

You can quit from the program in any of the following ways:

- Click **Close**  in the upper right-hand corner of the title bar of a window.  
—OR—
- From the **ACD/Labs** menu, choose **Close All**. This will attempt to close all ACD/Labs programs that are currently open, one after another.  
—OR—
- From the **File** menu, choose **Exit**. This will close only the currently open ACD/Labs program.

You will be prompted to save your work in the appropriate file formats depending on the window that you are quitting.

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## 2. Drawing Simple Structures

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### 2.1 Objectives

This chapter considers the basics of structure drawing, which occurs only in Structure Mode. The objective of this chapter is to give you an overview of the chemical drawing features of ACD/ChemSketch. From this chapter, you will learn how to:


- Draw atoms, bonds (single, double, triple, wedge, coordination, undefined, and Markush), as well as labels and polymers;
- Flip a drawn molecular structure;
- Select, rotate, and resize drawn structures;
- Generate stereo descriptors;
- Output the structure to a file, document, or printer; and
- Clear the screen.



### 2.2 Drawing Atoms, Bonds, and Labels

Drawing bonds and atoms is the basic activity in ACD/ChemSketch. Make sure that you are in Structure mode for all following actions:



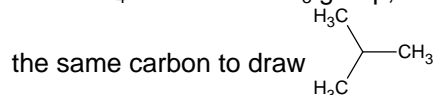
#### 2.2.1 Using the Draw Normal Tool

The Draw Normal tool  is the default tool when the program is started. In this mode, you can easily draw normal or branched chains and replace the drawn atoms with other atoms from the Periodic Table of Elements.

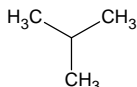
1. Make sure that the **Draw Normal** tool  is enabled on the Structure toolbar and that the **Carbon** atom  is selected on the Atoms toolbar.

2. Click in an empty space to draw CH<sub>4</sub>

3. Click CH<sub>4</sub> to add a —CH<sub>3</sub> group, creating CH<sub>3</sub>—CH<sub>3</sub> with a standard bond length. Click twice

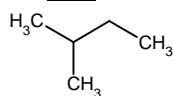


4. On the Structure toolbar, click **Set Bond Vertically**  and click any bond of the structure to rotate it to this orientation:

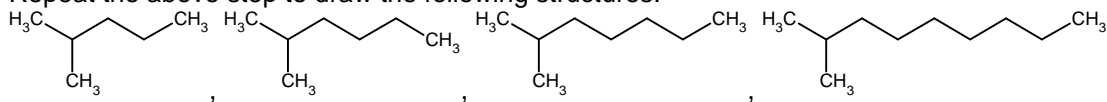


5. On the Structure toolbar, click **Draw Normal** .

6. Click the right-most carbon atom to draw



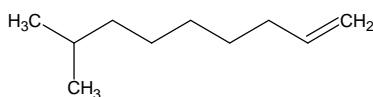
7. Repeat the above step to draw the following structures:



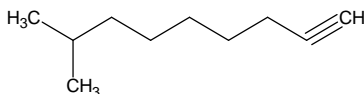
## 2.2.2 Double and Triple Bonds

Now we are going to draw double and triple bonds:

1. On the structure drawn, click the last bond to make it a double bond:



2. Click there again to place a triple bond:



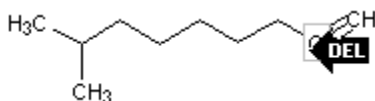
3. Click the triple bond to make it a single bond again.

## 2.2.3 Deleting Atoms Individually

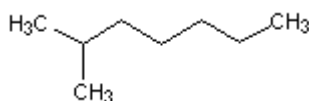
You can remove the superfluous atoms from the drawn structure:



1. On the General toolbar, click **Delete** .

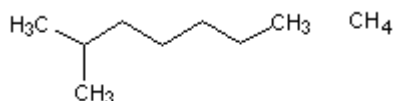
2. With the **Delete** tool active, click the atom as shown on the picture:



The structure now looks like this:




3. Now, click **Undo**  to reverse the changes and holding down CTRL click **Delete**  to delete the same atom:




As you can see, the end-atom attached to the deleted one is now retained.

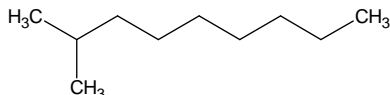
## 2.2.4 The Undo Command

Another important operation is how to “rescue” yourself from a change that, in retrospect, you wish you had not made.

1. Click **Undo** . This will cancel the last action performed and reset the workspace to exactly what it was before your last change.

**Note** As soon as **Undo** is executed, the **Redo** button (beside it) also becomes active.


2. Click **Undo**  several times until you return to the following structure:

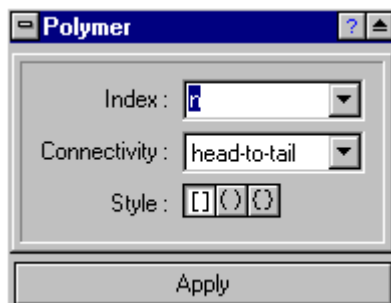


**Note** The **Undo** command can be repeated up to 50 times. When you begin to draw more complex structures or graphical objects, we recommend that you develop a habit of saving your work to a file after making several changes.

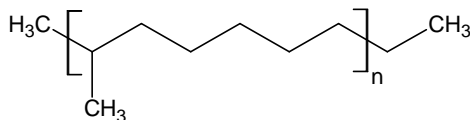
## 2.2.5 Polymers

ACD/ChemSketch allows you to draw polymeric structures:

1. On the Structure toolbar, click **Polymers**  to display the **Polymer** panel, and then change the settings as shown:




2. Select the area to be turned into a polymer by clicking or by dragging. As soon as the area is selected, the polymer appears in the workspace:



3. Leave the **Polymer Drawing** mode by closing this panel.

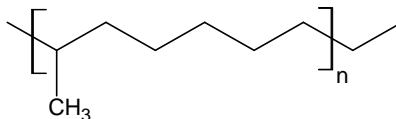
## 2.2.6 Pseudo Atoms

To create open-ended polymers and bent bonds, follow the steps:

1. On the Atoms toolbar, click **Pseudo Atom** .




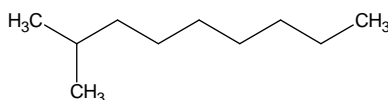
2. Click the end-atoms of the structure to replace them with empty atoms. You get an open-ended polymer:



### 2.2.7 Changing the Atom

To replace an atom with a new element whose button is not displayed on the Atoms toolbar, follow the steps:

1. Click **Undo**  several times until you return to the following structure or draw it:



2. On the Atoms toolbar, click **Periodic Table**  to display the **Periodic Table of Elements**.

Periodic Table of Elements																			
1 H																	9 <b>F</b> Fluorine Mass: 18.9984032 Valence: 1 Electron configuration: 2-7		18 He
2 Li	Be											13 B	14 C	15 N	16 O	17 <b>F</b>	Ne		
Na	Mg	3	4	5	6	7	8	9	10	11	12	Al	Si	P	S	Cl	Ar		
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe		
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn		
Fr	Ra	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg									
		* La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	D		
		** Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	T		

Characters : green-yellow gas, poisonous

Discoverer : 1886, H.Moissan, France

Name Origin : from 'fluere' (Latin) - to flow

Atomic Radius, A : 0.67      Ionization Potential, kJ/mol : 1681      Density, g/L : 1.7

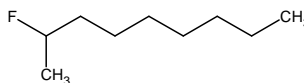
Electronegativity : 3.98      Electron Affinity, kJ/mol : 328      Melting Point, K : 54

Boiling Point, K : 85

General
NMR
Mass
Coloration


3. In the Periodic Table of Elements, click **Fluorine** , and then click **OK**. Note that **Fluorine** now appears on the Atoms toolbar.



4. Click the left-most carbon to replace it with a fluorine atom:

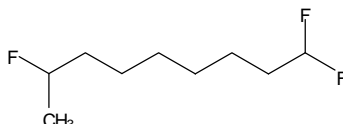


**Note** When you select new elements from the Periodic Table of Elements, the corresponding buttons are automatically added to the Atoms toolbar. To remove these buttons from the Atoms toolbar, double-click the Atoms toolbar and in the message box that appears, click **Yes**. This will remove all atom buttons except the default ones.



## 2.2.8 Using the Draw Continuous Tool



When the **Draw Continuous**  tool is active, bonds can only be drawn from the highlighted atom. To highlight an atom, click it. This mode is very convenient for “sprouting” new atoms from a selected atom.

1. On the Structure toolbar, click **Draw Continuous** . Alternatively, you can press the right mouse button to switch to this drawing mode.
2. Make sure that the **Fluorine** button  is pressed on the Atoms toolbar.
3. Click the right-most carbon in the drawn structure to select it. Click again to sprout fluorine from the selected carbon. Click twice on the same carbon again to sprout the second fluorine atom:



## 2.2.9 Using Mouse Drag

With either drawing tool, **Draw Normal**  or **Draw Continuous** , dragging from one atom to another draws a single bond between them. If you drag to or from an empty space, a new atom is inserted at the beginning or end of the drawn bond.

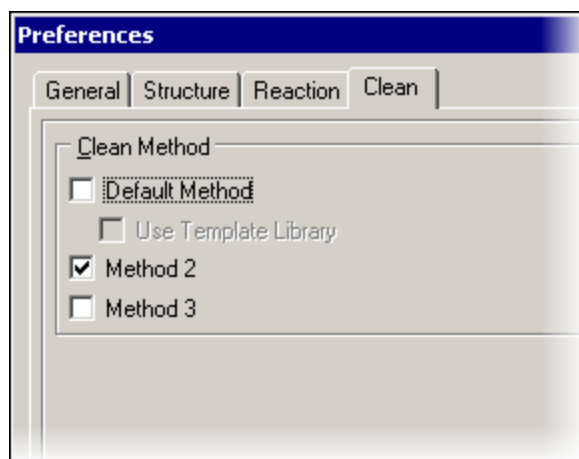
With either the **Draw Normal**  or **Draw Continuous** tool  active, point to one of the terminal carbons and drag to another terminal carbon to draw the following structure:


**Error! Objects cannot be created from editing field codes.**

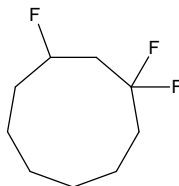
## 2.2.10 “Cleaning” the Structure

To standardize all the bond lengths and angles in the drawn structure, follow the steps:

1. From the **Options** menu, choose **Preferences**, and on the **Clean** tab of the **Preferences** dialog box, select the **Method 2** check box as shown in the picture:




2. On the Structure toolbar, click **Clean Structure** :

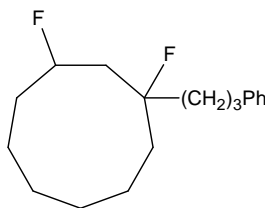



The **Clean** command not only standardizes all bond lengths and angles to make the structure look nice—it makes the drawn structures closer to being chemically correct. For acyclic fragments, for example, it places the bonds near the  $sp^2$  carbons at  $120^\circ$  angles and the bonds near the  $sp$  carbon at  $180^\circ$  (linear). If you draw geometrical and stereoisomers, the **Clean** command standardizes their bond lengths and angles while retaining all of their structural significance.

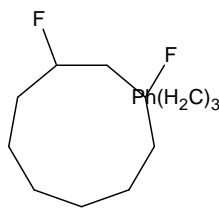
### 2.2.11 Editing Atom Labels


The **Edit Atom Label**  tool allows you to substitute terminal atoms with shorthand abbreviations. Using the structure cleaned in Section 2.2.10, follow the steps below:


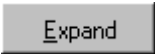
1. On the Atoms toolbar, click **Edit Atom Label** , and then click the right-most fluorine atom on the drawn structure.
2. In the **Edit Label** dialog, type **(CH<sub>2</sub>)<sub>3</sub>Ph** and click **Insert**. Note that the label is inserted in the desired position and the indexes are automatically subscripted:

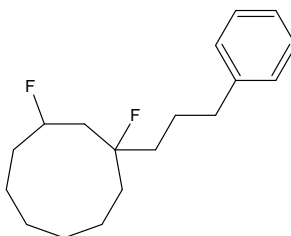


3. Click **Change Position** , and then click the label to invert it:




**Tip** If you hold down SHIFT and click the label with the **Change Position**  tool active, the connection point of the label will be changed.

4. With the **Edit Atom Label**  tool active, click the obtained shorthand abbreviation to open the **Edit Label** dialog box again. Then click **Expand**  to obtain the following structure:

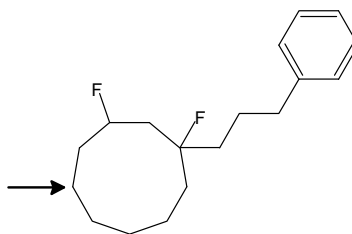


**Important** Only group abbreviations that substitute terminal atoms as atom labels can be expanded by clicking **Expand**.

## 2.2.12 Draw Chains Tool





Using the **Draw Chains**  tool, you can easily draw short or long chains by clicking and dragging.

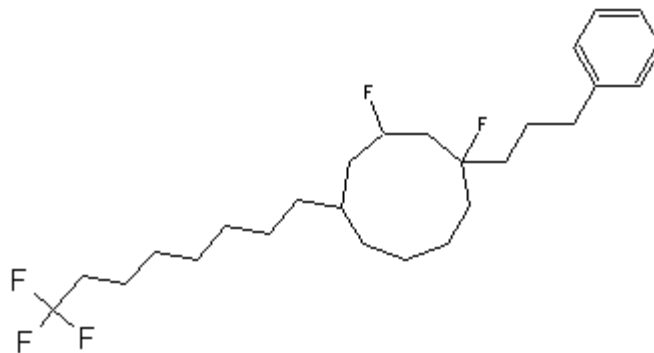
1. On the Structure toolbar, click **Draw Chains**  and point to the atom indicated by the arrow:





2. Drag to the left side, a carbon chain is created. Note the carbon counter (C #) located beside the mouse arrow changes with each carbon added or removed. Continue until the counter reaches C 8, then release the mouse button to finish the chain:

**Error! Objects cannot be created from editing field codes.**



3. With the **Draw Chains**  tool active, on the Atoms toolbar, click **Fluorine** , and then click the left-most CH<sub>3</sub> group three times to sprout three fluorine atoms. Then click **Select/Move** , select these three fluorine atoms, and click **Clean Structure** . The structure became as follows:



**Note** Dragging with the **Draw Chains**  tool active draws a chain where the bonds are set at an angle of 120° to each other. However, holding down CTRL while dragging with the **Draw Chains**  tool active produces a chain where the bonds are set at an angle of 180° to each other.

## 2.3 Clearing the Screen

If you have to clear the screen, you can do one of the following:

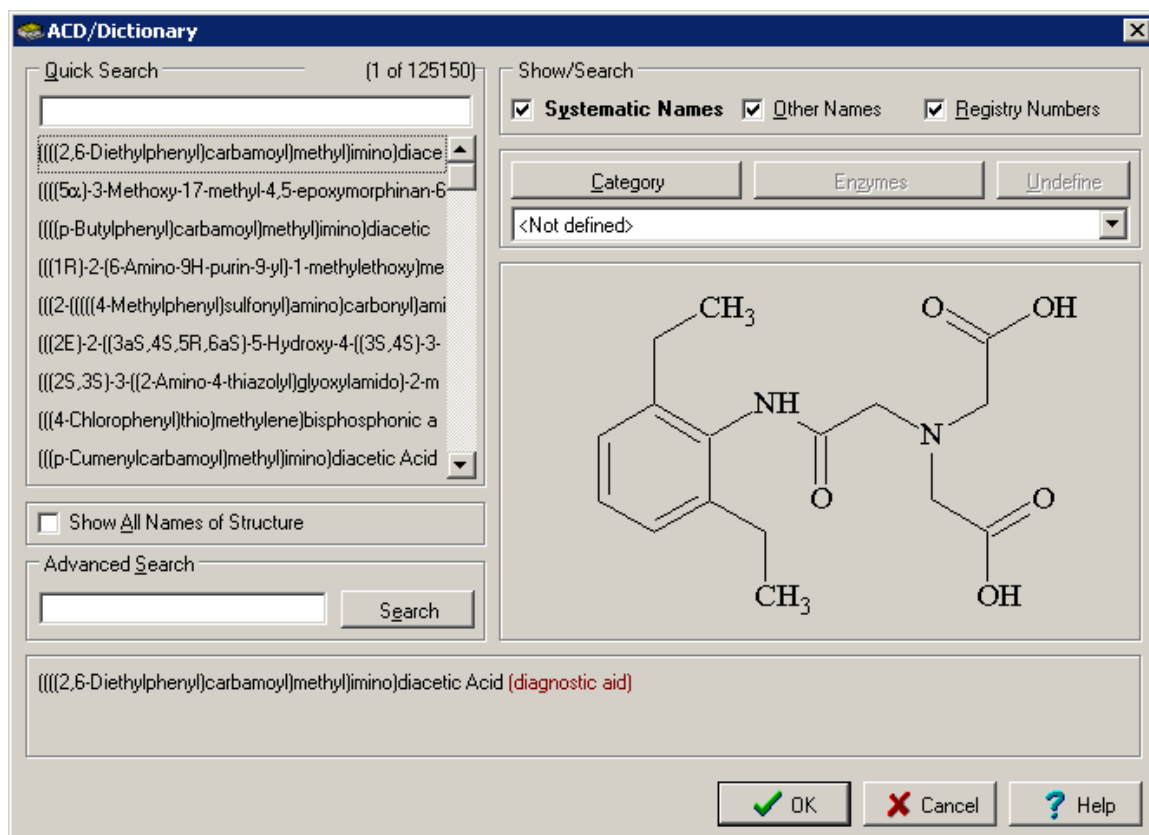
- From the **File** menu, choose **New**. This will open a new empty document.
- Click **New Page**  from the upper left set of buttons to insert a new empty page.
- From the **Edit** menu, choose **Select All** and then from the **Edit** menu, choose **Delete**.
- Press CTRL+A to select all the objects on the page and then press DELETE.
- On the General toolbar, click **Delete** . Click an empty space away from the drawn structure to select all of the structures, and then click any structure to clear the entire screen.

Clear the screen using one of the aforementioned ways.

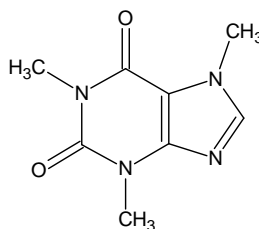
## 2.4 Using ACD/Dictionary—**Commercial version only!**

ACD/Dictionary allows you to find the molecular structure for common drug names, but this module is only available in the commercial version of ACD/ChemSketch. If you are using the freeware version and the ACD/Dictionary is not available, skip this section.

1. To display the ACD/Dictionary, on the Reference toolbar, click **ACD/Dictionary** .



2. Right-click the title bar of the dialog box, to display the shortcut menu. Make sure that **Copy Structure with Name** is not selected.
3. In the **Quick Search** box, type *caffeine*. As you type the list scrolls to display the corresponding names. As soon as the required name is visible in the list, click it to select. The corresponding structure is displayed in the preview area to the right.
4. To place the selected compound onto the workspace, click **OK**.
5. The structure shadow is attached to the cursor. Point to an empty space and click to insert the structure:

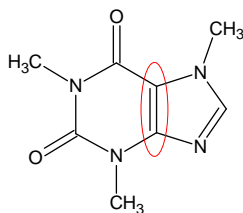



**Note** For more details on the ACD/Dictionary options, refer to the *ACD/Dictionary User's Guide* located in the ACD/Labs documentation folder (\\DOCS\\DICT.PDF).

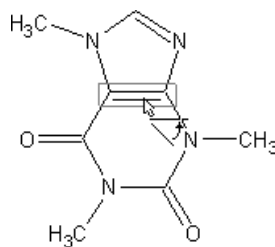
## 2.5 Flipping Structures


You can rotate or flip the entire structure with a single button click using a set of tools on the Structure toolbar.

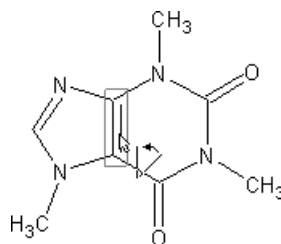
1. Take the structure of caffeine from the Dictionary as described in the previous section or draw it manually. We are going to rotate the structure relative the double bond indicated with red line in the image below:




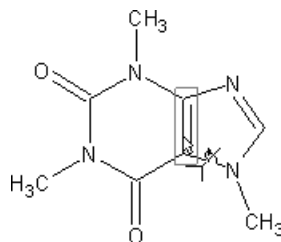
2. Click **Set Bond Horizontally**  and then click the bond to set it horizontally, rotating the rest of the structure correspondingly. Repetitive clicking the bond with this tool will rotate it around the clicked bond:





3. Click **Set Bond Vertically**  and then click the bond to set it vertically, rotating the rest of the structure correspondingly.



4. Click **Flip on Bond**  and then click the bond, the structure will rotate around the bond clicked:

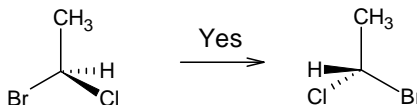


5. Select the entire structure (or fragment) first. Click **Flip Top to Bottom**  and the selected structure or fragment (or if nothing is selected, all the drawn structures) will rotate from top to bottom.
6. Click **Flip Left to Right**  to flip the selected structure or fragment (or if nothing is selected, all drawn structures) from left to right.

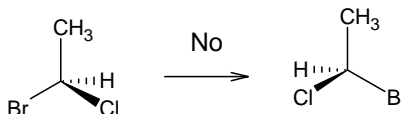
**Note** Applying the **Flip** tools might change the stereo configuration. To control this, from the **Options** menu, choose **Preferences**, and then switch to the **Structure** tab. The **Keep Stereo Configuration on** area controls whether the program will remember the “true” 3D arrangement of the structure:

Keep Stereo Configuration on : ☐ Clean ☒ Flips

We recommend that the **Flips** check box be selected. In this case, the structure before the flip is the same as the structure after the flip, although its representation has changed:



If the **Flips** check box is cleared, the structures before and after the flip are enantiomers:



## 2.6 Output

As soon as you have drawn one or more structures you can save them to a file, print them, or insert them into the other applications such as MS Word, Excel, etc. You can also use the drawn structure(s) to try out the ACD/I-Lab services (refer to the *ACD/I-Lab User's Guide* located in the ACD/Labs documentation folder, \\DOCS\\LAB.PDF).

### 2.6.1 Saving a ChemSketch (.SK2) File

Let us save the document with the structures created in previous sections in the default proprietary ACD/Labs format,<sup>1</sup> as a file which we will call EXAMPLE1.SK2.

1. From the **File** menu, choose **Save**.

<sup>1</sup> The details for the .SK2 file format are spelled out in the .SK2 Format document available from <http://www.acdlabs.com/download/#misc>.

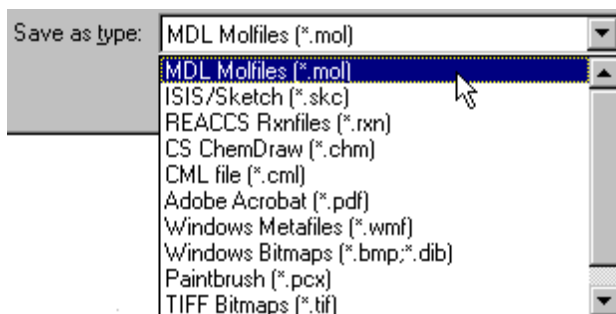


2. In the dialog box that appears, specify the name and location of the file to which the work should be placed. Click **OK**.

### 2.6.2 Saving a Structure to a MDL Molfile

A standard format shared by many programs is the molfile format, developed by MDL, Inc. Note that it will not retain graphical images, text, etc. It *only* retains the molecular structure.

1. Select the structure you want to save as a molfile.
2. From the **File** menu, choose **Export**. In the **Save As Type** box, select **MDL Molfiles (\*.mol)**:

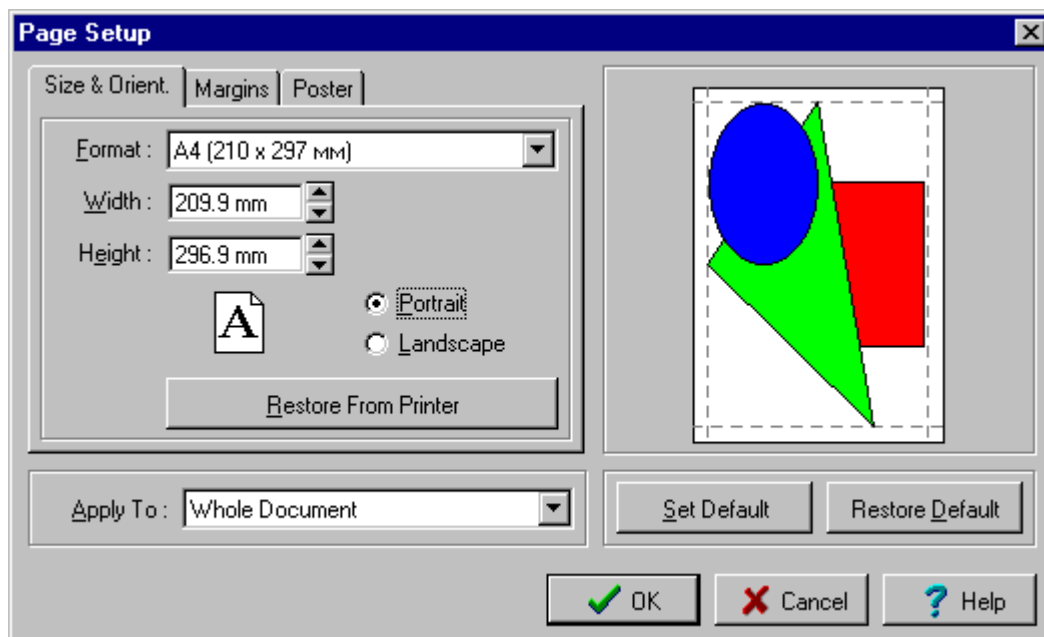


3. Specify the name and location of a file and click **Save**.


### 2.6.3 Printing

Another way to preserve your work is to print a report. Before starting printing, verify the page setup settings.

1. From the **File** menu, choose **Page Setup** to display the dialog box where you can specify the paper size, orientation, margins for the page, and if you wish set options for the poster (more details on the poster creation can be found in Section 10.3):




2. Click **OK** to save settings.
3. On the General toolbar, click **Full Page**  to see how the page will look on a printout.

4. If necessary, move the objects on the page to arrange them properly.
5. From the **File** menu, choose **Print** or, on the General toolbar, click  to display the **Print** dialog box where you can specify the number of copies to be printed. Click **Print**.

## 2.6.4 Embedding the Structure in a Document

Sometimes you need to insert the structure into a report written in applications other than ACD/ChemSketch (e.g., Word document, Excel spreadsheet, etc.).

1. Select the required structure(s).
2. To copy the selection to the Clipboard, on the General toolbar, click **Copy** .  
–OR–  
From the **Edit** menu, choose **Copy**.  
–OR–  
Press CTRL+C.
3. Switch to the application where you want the structure(s) to be inserted and paste using the **Paste** command of that application.

**Important** When pasting structures copied from ACD/ChemSketch to other applications (e.g., Microsoft Excel), the structure may be represented as a set of numbers and figures (as an MDL molfile). To place a picture of the structure, use the **Paste Special** command in the application you are pasting to. Among the paste options choose either the **ACD ChemSketch 2.0 Object** or **Picture** option. The former inserts the structure as an OLE object thus allowing you to edit the inserted structure via ACD/ChemSketch by double-clicking the picture.

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## 3. Drawing More Complex Structures

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### 3.1 Objectives



Now that you have studied the basics of structure drawing described in Chapter 2 you may want to draw more complex structures using the advanced tools of ACD/ChemSketch.

In this chapter, you will learn how to:

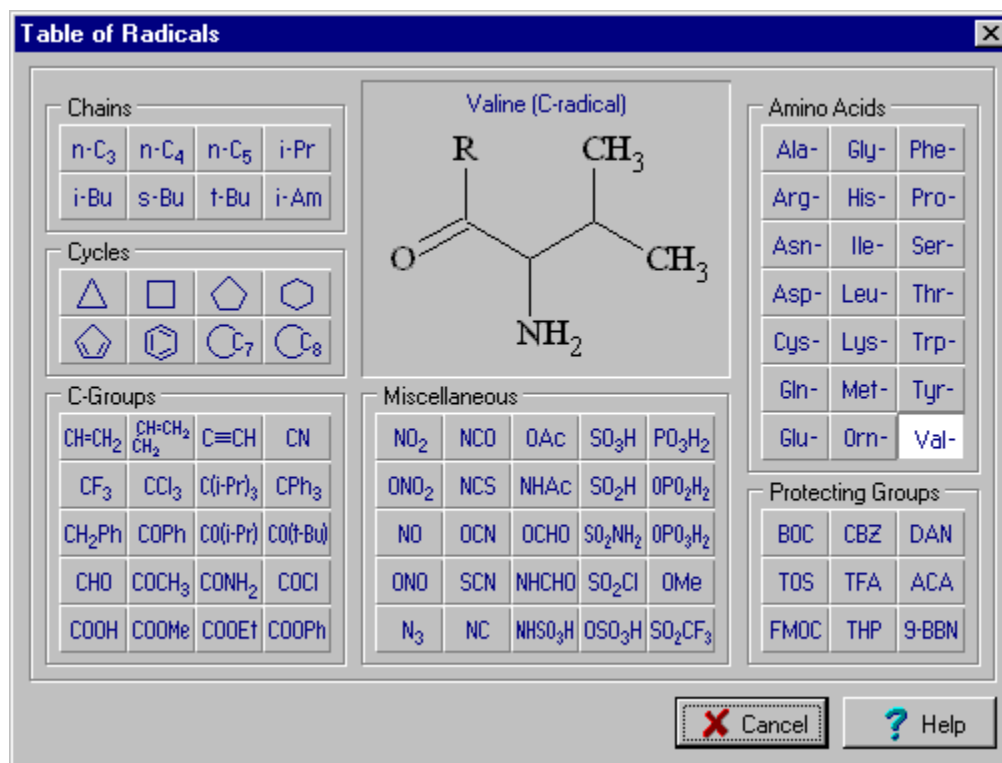
- Use the Table of Radicals to draw typical chemical fragments;
- Quickly draw ring structures;
- Delete and replace atoms;
- Set double and triple bonds;
- Set an atom's charge, draw cations and anions; and
- Change various atomic properties.




### 3.2 Using the Table of Radicals

The Table of Radicals includes pre-drawn structures of amino acids, their protecting groups, as well as nucleotides and other frequently used radicals.

1. On the General toolbar, click **Save File** , then click **New Page**  to start new drawing from a new page of the same document.

2. On the References toolbar, click **Table of Radicals**  to display the radicals:




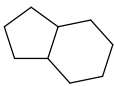


3. Click **Cyclohexane** —a **Cyclohexane** button is now located and currently selected on the References toolbar on the right side of the screen. Right-click to hide the template shadow—we are going to use it later.
4. Repeat these steps for **Cyclopentane**  and **Carboxyl** .

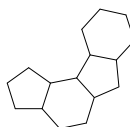
**Note** When you select new radicals from the **Table of Radicals**, the corresponding buttons are automatically added to the References toolbar. To remove these buttons from the References toolbar, double-click the References toolbar and, in the message box that appears, click **Yes**.

### 3.3 Using Ring Structures

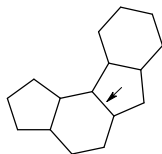
Now we'll draw hexadecahydrocyclopenta[*c*]fluorene-3,4,5,7,8,9-hexacarboxylic acid.

1. On the References toolbar, click **Cyclopentane** .
2. Click in the workspace to paste a five-membered ring.
3. On the same toolbar, click **Cyclohexane** . Now point to the indicated bond  and then click to create the following structure: 

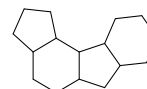
4. Repeat these steps to create the following structure;



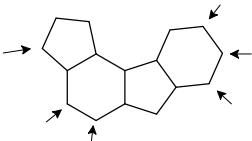
5. On the Structure toolbar, click **Set Bond Vertically**  then click the indicated bond



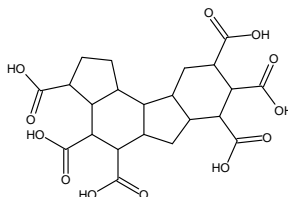
to rotate the structure around this bond to obtain the following:



6. On the References toolbar, click **Carboxyl** .

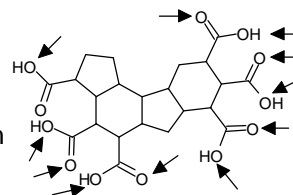
7. Click the atoms indicated on  to sprout carboxyl groups from them to

obtain:

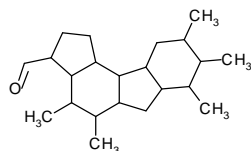


### 3.4 Deleting Atoms and Fragments

We are going to delete the atoms indicated by the arrows on



to draw



You can do this in two ways: delete each atom individually (covered in Section 2.2.3) or delete several atoms simultaneously.

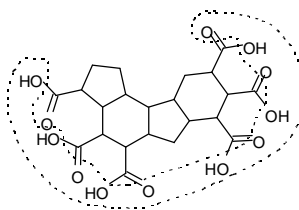
#### 3.4.1 Deleting Several Atoms Simultaneously

In this section, you will learn how to delete all the required structural elements at once:


1. On the Structure toolbar, click **Lasso On/Off**  to enable the **Lasso** selection mode .

Note **Select/Move**  becomes active.

2. Drag to include all of the specified atoms in the closed Lasso line to select them:





**Note** The dotted path on this picture shows the suggested path enclosing the desired groups, and it will not appear as such in your workspace. Only the atoms within the lassoed space are selected.

3. On the General toolbar, click **Delete**  and click any of the highlighted atoms to delete all of them simultaneously.

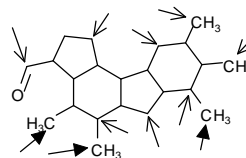
-OR-

On the keyboard, press DELETE.

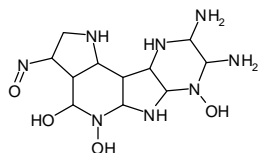
**Note** You can select atoms, bonds, and fragments in two different ways, by using either the **Lasso** selector  or the **Rectangle** selector . To deselect all fragment(s), click anywhere in the empty space.



### 3.5 Replacing Atoms

Now we will replace the atoms indicated with arrows on



to draw



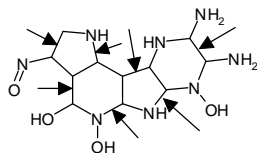
1. On the Atoms toolbar, click **Nitrogen** , and then click all the carbons denoted by an open-head arrow on the above structure.
2. On the Atoms toolbar, click **Oxygen** , and then click the three Carbons denoted by a solid-head arrow.

**Note** You cannot replace atoms with the **Draw Continuous**  tool (see Section 2.2.8).

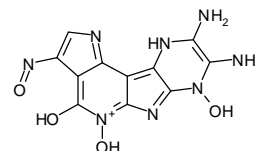
### 3.6 Setting Double and Triple Bonds


This section will familiarize you with drawing double and triple bonds:

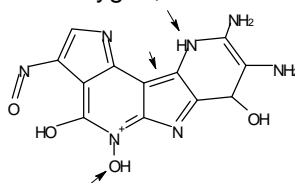
1. With any of the **Draw Normal** , **Draw Continuous** , or **Draw Chains**  tools active, click the bonds indicated on



to set double bonds:



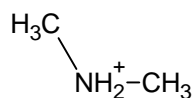
2. Using the **Change Position** button , the structure's appearance can be "fine-tuned". Click this button, and then click the indicated hydrogens and double bonds. Note the movement of hydrogen around the nitrogen and oxygen, and the double bond around the single bond:



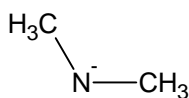
3. On the General toolbar, click **Save File** , then click **New Page** .

### 3.7 Setting Charges and Defining Anions and Cations

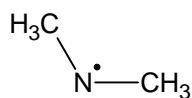
In this section, we will draw the following set of structures:



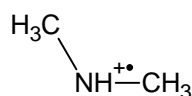
**cation**



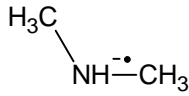
**anion**



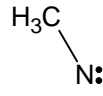
**free radical**



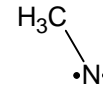
**positive radical ion**





**negative radical ion**

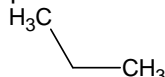



**singlet biradical**

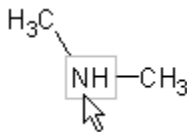



**triplet biradical**






1. On the Atoms toolbar, click **Carbon**  and make sure that the **Draw Normal**  tool is active. Click three times at the same point to draw the following structure:




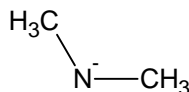
2. On the Atoms toolbar, click **Nitrogen** , and then click the middle carbon to replace it with a nitrogen:




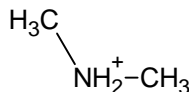
3. On the Atoms toolbar, click the bottom right triangle of **Increment (+) Charge**  to expand it to the following buttons:



	Increment (+) Charge
	Decrement (-) Charge
	Radical
	Positive Radical Ion
	Negative Radical Ion


4. Click **Decrement (-) Charge**  and then click the NH group to make an anion:

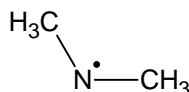



5. Right-click to switch to the **Increment (+) Charge** tool (or choose  from the group of buttons) and click twice to make a cation:

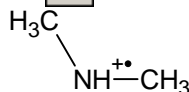



**Note** When you use the **Charge** buttons,  or , to change the charge of a nonmetal, the corresponding number of hydrogen atoms is automatically added to it, or removed from it, to preserve proper chemical valency. If you change the charge of a metal, the charge is changed in increments or decrements in accordance with the next chemically valid charge of the corresponding ion. (You can view common valences used in the **Periodic Table of the Elements**.)

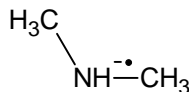
6. Click **Radical**  from the group of buttons shown in step 3 above and click the NH<sub>2</sub> group to draw a free radical:



7. Right-click in an empty part of the workspace to quickly switch to the **Positive Radical Ion** tool or choose the corresponding button  and click to draw the positive radical ion:



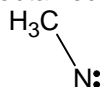
8. Right-click in an empty area of the workspace to switch to the **Negative Radical Ion**  tool and click to draw the negative radical ion:



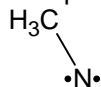
9. On the top General toolbar, click **Delete**  and click the right CH<sub>3</sub> group to delete it.



10. From the group of buttons in step 3, click **Radical**  and click the NH group several times until the following singlet biradical is obtained:



11. Click again with the radical tool until the triplet biradical is displayed:







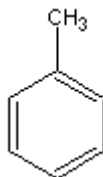
12. On the General toolbar, click **Save File** , then click **New Page** .




### 3.8 Markush Bonds

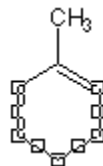
To denote structures with an undefined attachment point, use one of the Markush bond tools:





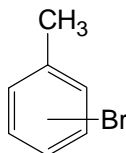
1. In the **Table of Radicals** , click **Benzene** , and then click an empty area of the workspace.
2. On the Atoms toolbar, click **Carbon** . Note that the **Draw Normal**  tool is automatically activated.
3. Click the topmost atom of benzene to sprout CH<sub>3</sub>:



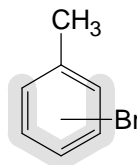
4. On the Atoms toolbar, click **Bromine** .
5. Using the **Select/Move**  or **Select/Rotate/Resize**  tools select five lower atoms of the structure:



6. On the Structure toolbar, click either **Markush Bond**  or **Markush Bond with Shadow**  tool. The selected element connected by the Markush bond appears:





OR

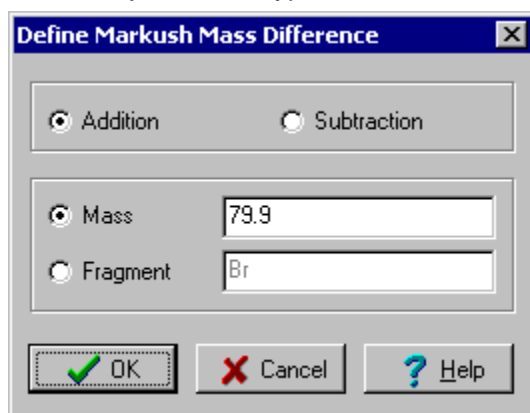


On this structure, Br might be connected to any of the five carbon atoms of toluene. ACD/ChemSketch allows you to highlight this phenomenon by pointing to the variable attachment point of the Markush bond.

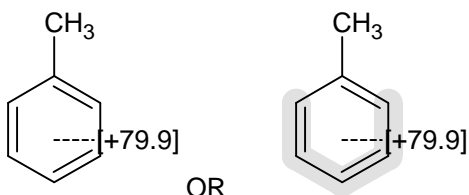
### 3.8.1 Markush Bond with Added or Removed Fragment

Starting with version 9.0, you can draw structures with the attached mass or formula difference values, instead of the added or removed structural fragments itself. This special type of Markush structures is useful for designation of metabolic or mass-spectral transformations of chemical structures.

1. To apply this option, draw toluene as described above and select five lower atoms of the structure.
2. On the Structure toolbar, click **Markush Bond with Added or Removed Fragment** button: either  or .
3. In the **Define Markush Mass Difference** dialog box that appears, select the **Addition** and **Mass** options, and then, in the adjacent box, type 79.9:



4. Click **OK**. You can see one of the following structures:

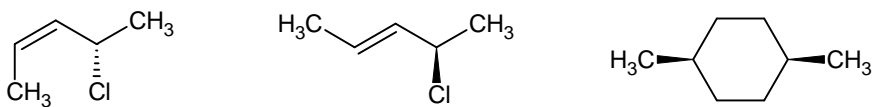




5. On the General toolbar, click **Save File** , then click **New Page** .

## 3.9 Generating Stereo Descriptors

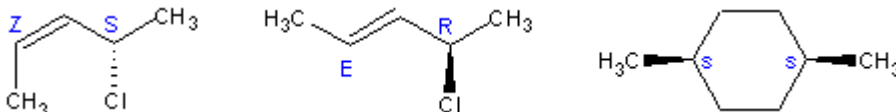
ACD/ChemSketch allows you to generate stereo descriptors for chiral and pseudo chiral centers, and for a double-bond configuration.

1. Draw the following set of structures using the tools described above:



**Tip** To draw a stereo bond, on the Structure toolbar, click **Up Stereo Bonds**  or **Down Stereo Bonds** . Then change a bond to a stereo bond by clicking the desired bond on the chemical structure, or drag from the atom to an empty space, or simply click an existing atom (if the existing atom is of the same type as that currently active on the Atoms toolbar). To change the direction of the stereo bond, click this bond as many times as you need.

2. Select all of the structures.
3. On the **Tools** menu, point to **Generate**, and click **Stereo Descriptors** (you can do this both in Structure and Draw modes). Stereodescriptors appear on the selected structure(s) near the corresponding chiral center or double bond:



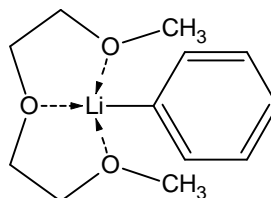
4. The following stereodescriptors are available:
  - **S** and **R** describe a chiral center configuration.
  - **E** and **Z** describe a double-bond configuration.
  - Small **r** and **s** describe configurations of pseudo chiral centers.
5. To change the color of stereo descriptors, from the **Options** menu, choose **Preferences**.
6. In the **Preferences** dialog box that appears, switch to the **Structure** tab, and then select the appropriate color in the **Auto/Manual Numbering Color** box. The next time you generate stereodescriptors, the defined color will be used.

**Note** If no structure(s) is(are) selected in the workspace, stereodescriptors are automatically generated for all structures on the current page which have stereo centers or double bonds for which Z/E or R/S isomerism is possible.

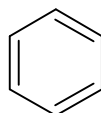
7. On the General toolbar, click **Save File** , then click **New Page** .

### 3.10 Drawing Coordination Bonds

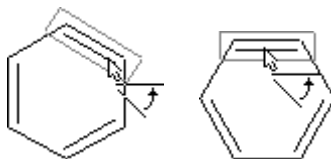
There are numerous ways to draw coordinating bonds. ACD/ChemSketch allows you to draw four different types. We are going to draw the following structure:






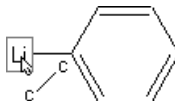
1. Using the **Table of Radicals** or the buttons on the Reference toolbar, paste the benzene ring to the workspace:





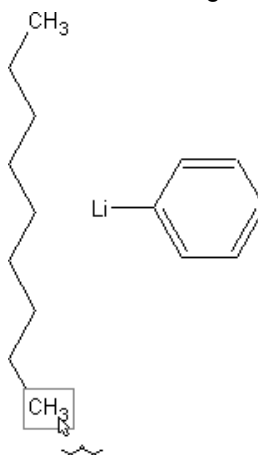
2. On the Structure toolbar, click **Set Bond Horizontally**  and then click the bond as shown below to rotate the ring:





3. Activate the **Draw Normal**  tool and, in the **Periodic Table** , click **Lithium**  and click **OK**. Point to the leftmost group of atoms in the ring and drag from it to sprout **Li**:

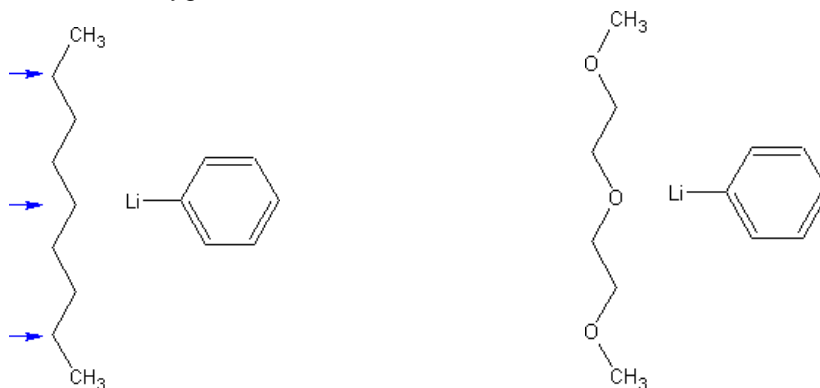




4. Click **Carbon**  on the Atoms toolbar and then click **Draw Chains** . Drag in an empty space so that the chain contains 9 elements. When dragging, move the chain so that it is located to the left of the drawn structure not touching it:

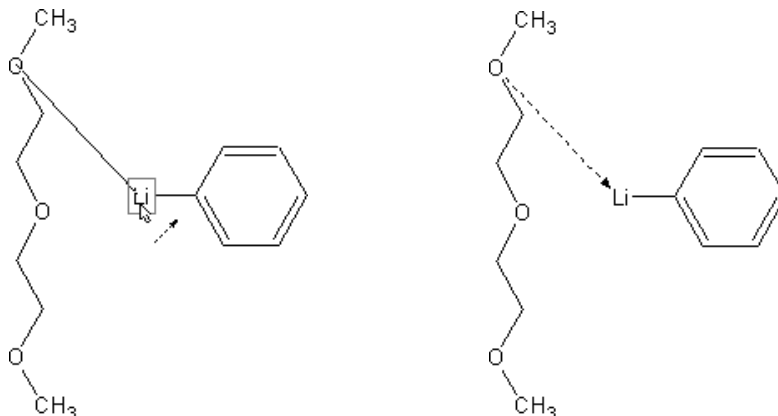


**Note** If in the **Preferences** dialog box (**General** tab), the **Informative Cursor** option is selected, you will see the number of elements hang near the cursor when you draw the chain.

5. Now right-click in the workspace to switch to the **Draw Normal**  tool and, on the Atoms toolbar, click **Oxygen** . Click the buttons indicated with arrows in the picture below to replace them with the oxygen atoms:

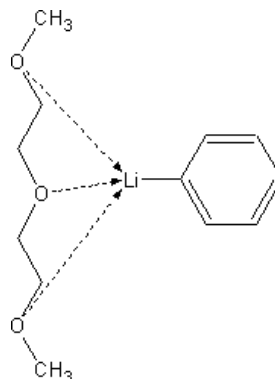


6. On the Structure toolbar, click the white triangle of the **Coordinating Bonds** button  and choose the **Coordinating (Dashed Arrow) Bonds** button .
7. Drag from one of the oxygen atoms to the Li atom to connect them with the coordinating bond. As you release the mouse button, the bond appears:

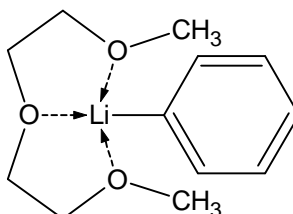


**Note** If the bond arrow is directed the wrong way, point to the bond so that it is highlighted and click to change the direction.

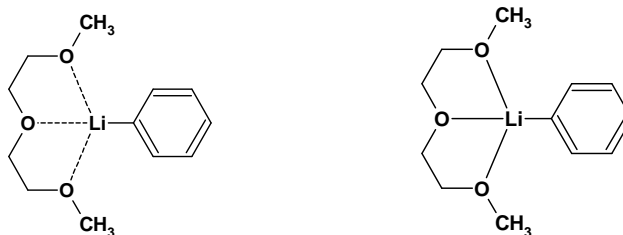
8. In the same manner, drag from other oxygen atoms to Li to draw other bonds:



9. Click **Clean Structure**  to standardize all the bond lengths and angles:



To practice the bond drawing, you can try the following structures:

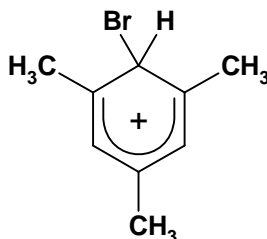




**Note** Even looking as common bonds, coordinating bonds do not affect valences and charges of connected atoms. All the types are coded in the same way, so all the three drawings above describe the same structure.

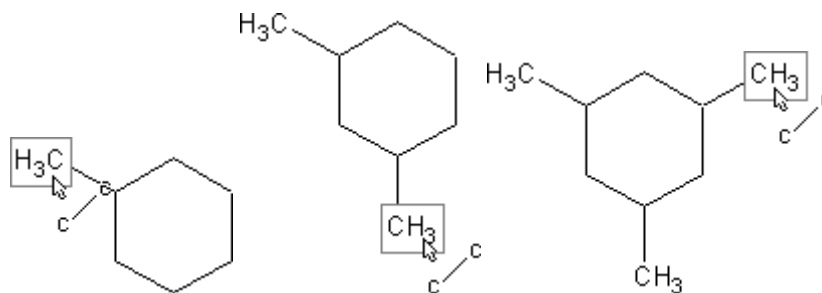
10. On the General toolbar, click **Save File** , then click **New Page** .



### 3.11 Delocalized Charges and Curves

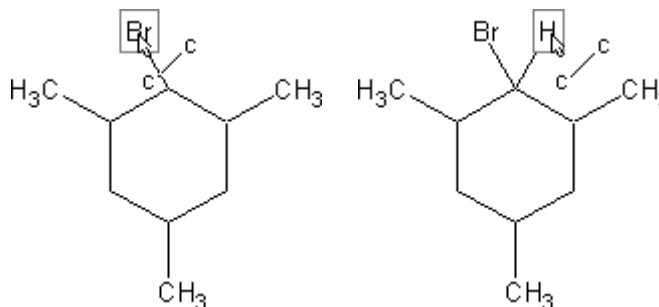
The delocalized bonds and charges can be used to draw reaction intermediates, delocalized charges and organometallic structures with multicentral coordination. To practice this type of bonds we are going to draw the following structure:




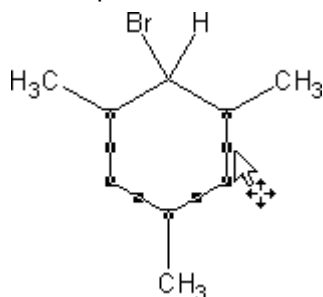
1. On the Reference toolbar or from the **Table of Radicals**, choose **Cyclohexane**  and paste it into the workplace.
2. On the Atoms toolbar, click **Carbon** . By dragging from the atoms in the ring, sprout the **CH<sub>3</sub>** groups:



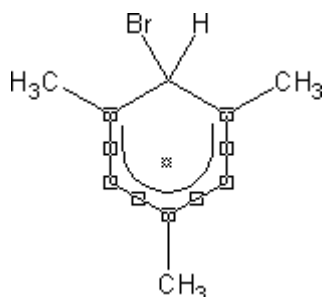
3. If **Bromine**  is not available on the Atoms toolbar, click **Periodic Table**  and find it in the table. If it is available—click it. Drag from the upper atom of the ring to sprout a new bond.
4. Click **Hydrogen** and drag from the same atom to sprout one more bond:




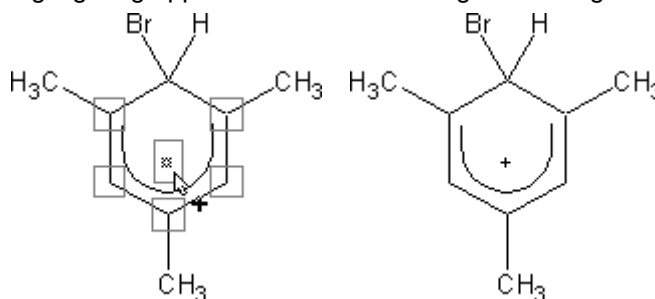
5. Activate the **Select/Move**  tool. Hold down SHIFT and click one by one the bonds so that they become selected as shown on the picture below:



6. On the Structure toolbar, click **Solid Delocalization Bond**  to apply it to the selected bonds:



7. Click **Increment (+)Charge**  on the Atoms toolbar, point to the center of the delocalized bonds so that the highlighting appears and click to change the charge to "+":



**Note** If you want to make the plus sign more prominent, you can change its size by changing the properties as described in Section 3.13 below.

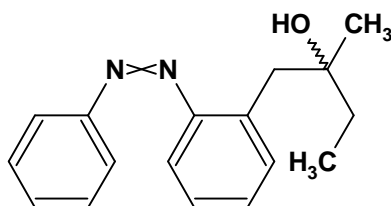
Now try to draw the following structure yourself to practice the delocalized bond drawing:





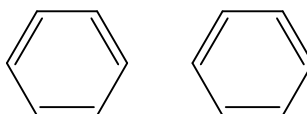
8. On the General toolbar, click **Save File** , then click **New Page** .

### 3.12 More Bond Types


In this section, we are going to draw the following structure that contains undefined double and single stereo bonds which denote that configurations of double bond or chiral center is not known or not taken into account.

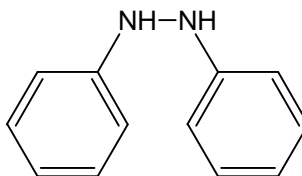



1. On the Reference toolbar, use either **Benzene**  or **Table of Radicals**  to insert two structures as displayed below:

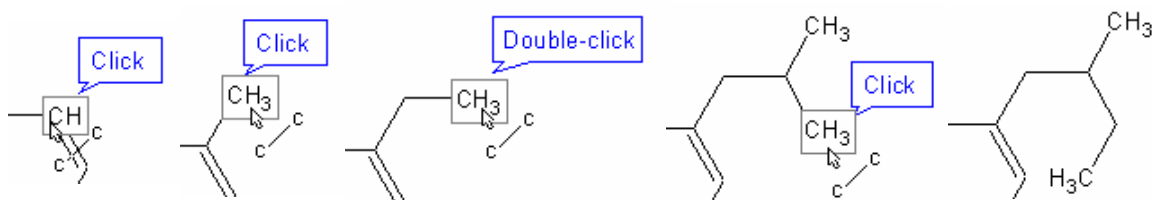


**Tip** On the Structure toolbar, click **Set Bond Horizontally**  to rotate the inserted templates.


2. On the Atoms toolbar, click **Nitrogen**  and by dragging and releasing connect two rings in the following way:

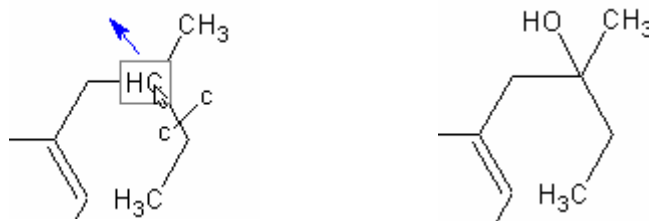




3. On the Atoms toolbar, click **Carbon**  and by subsequently clicking the atoms as shown below, add one more fragment:






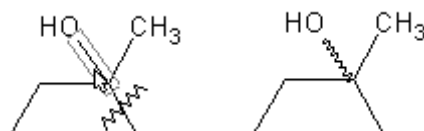
4. On the Atoms toolbar, click **Oxygen**  and drag from the indicated atom left and up to sprout a group:



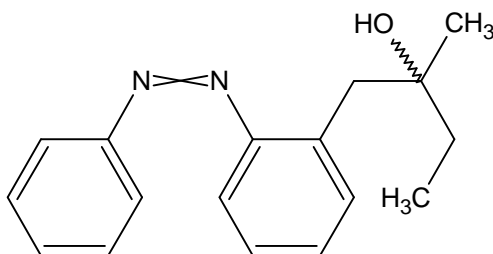
5. On the Structure toolbar, click the white triangle of the **Undefined Stereo Bond**  button to display more bond types. Click **Undefined Double Stereo Bond**  to select it. Click the indicated bond to replace it with the another type:



6. From the same group of buttons on the Structure toolbar, click **Undefined Stereo Bond**  and click the structure to replace as indicated:

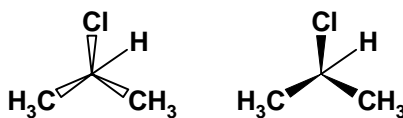


As a result, the following structure should be displayed:

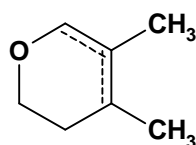


To practice the drawing of other bond types, try to draw the following structures:

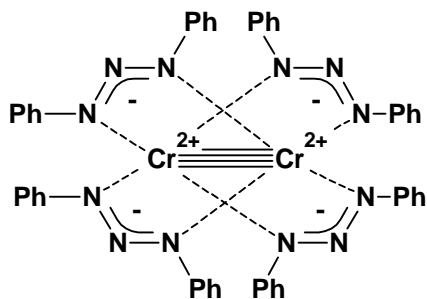
- Hollow wedges are used sometimes to describe spatial arrangement of atoms. Hollow bonds are equal to more common up stereo bonds:



- Delocalized and partial order bonds can be used to describe delocalization of double bonds, tautomeric or aromatic structures.



- Quadruple bonds are used to describe the structure of some organometallic complexes.

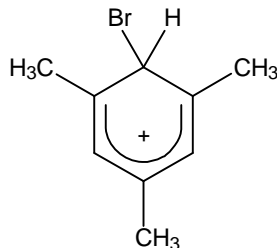



7. On the General toolbar, click **Save File** , then click **New Page** .

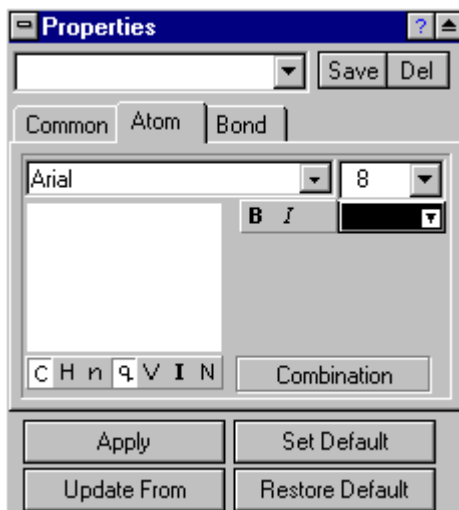
### 3.13 Changing Atom Properties

If you want to display the valency or the isotopic mass of an atom of a structure drawn in ACD/ChemSketch—or even change the typeface or the size of the atom identification—you should use the **Properties** panel.

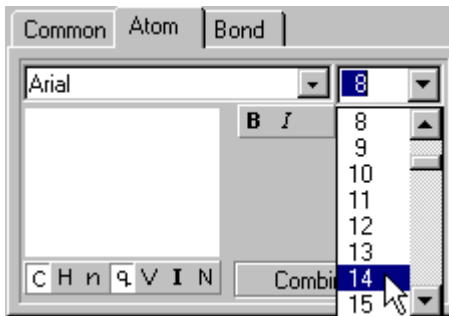
You can use the structure drawn in Section 3.11. We are going to change the size of the plus sign and make the visible atom symbols bold:



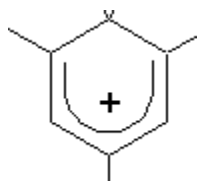
1. On the Structure toolbar, click **Select/Move** .
2. Point to the plus sign and double-click. This will make the **Properties** panel appear. Switch to the **Atom** tab:





3. As you can see, the buttons below the preview area allow you to change the atom symbol and charge **C H n q V I N**. For font sizes, select 14.



4. Click **Apply** to view the result on the selected element:



5. By selecting other structure parts or the whole structure and double-clicking the selection, try modifying various attributes in the **Properties** panel.
6. On the General toolbar, click **Save File** , then click **New Page** .

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## 4. Advanced Structures, SMILES and InChI Notations, Reaction Schemes



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### 4.1 Objectives

This chapter is the next step to drawing even more sophisticated structures. Two kinds of optimization are covered: optimizing for display purposes (2D) and optimizing according to a simple force-field model (3D). If you are using ACD/ChemSketch for the first time, it is recommended that you do the exercises described here only after completing the previous chapters.

In this chapter, you will learn how to:

- Draw structures of cyclic Alkanes and Peptides using the **2D optimization** (Clean Structure)  tool;
- Convert structures to SMILES format and vice versa;
- Convert structures to InChI string and vice versa
- Use the **3D Optimization** tool  for drawing “spectacular” 3D structures of Bicyclo[2.2.2]octane, triptycene, cubane, and dodecahedrane;
- Draw reaction schemes and reflect the reaction conditions on it;
- Map reactions; and
- Use the Reaction Calculator—*Commercial version only!*.

### 4.2 2D-Optimization

The **Clean Structure**  tool can be considered to be a 2D-optimization of the drawn structure, *i.e.* redrawing and resizing it to standardize all the bond lengths and angles. Using this tool you can easily draw a perfect structure. Some examples are put below:



#### 4.2.1 Creating the Structure of Cyclic Alkanes

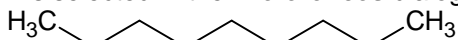


This section is based on the movie **cycloalk.exe** which can be downloaded from our Web site or found in the \\MOVIES folder.

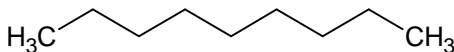
Using the following technique you can quickly draw cyclic alkanes perfectly. Here's how to draw a cyclononane:




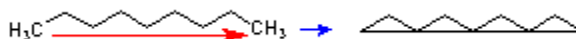
1. On the Atoms toolbar (Structure mode), click **Carbon** .
2. On the Structure toolbar, click **Draw Chains**  and drag in the workspace to draw a 9-member chain. Note that the informative cursor shows the number of atoms in the chain if the **Informative Cursor** check box is selected in the **Preferences** dialog box (**General** tab).



3. On the Structure toolbar, click **Flip Top to Bottom**  the structure is turned upside down:



4. Right-click to quickly switch to the **Draw Normal**  tool and drag from one end atom to another in order to connect them with a bond.



5. Click **Clean Structure**  to obtain the following structure:




! Try to draw C<sub>10</sub>- and C<sub>8</sub>-rings using the above technique.

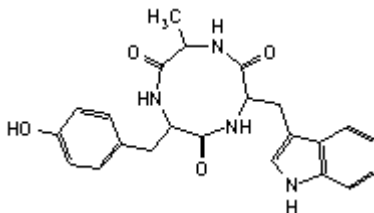
6. On the General toolbar, click **Save File** , then click **New Page** .


## 4.2.2 Creating the Structure of a Cyclic Peptide






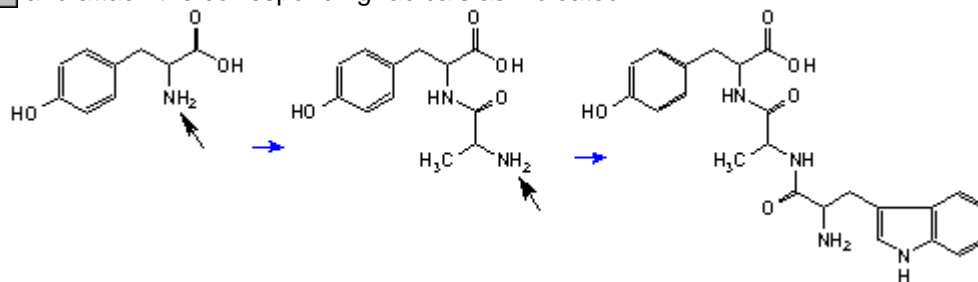
This section is based on the movie **pept.exe** which can be downloaded from our Web site or found in the \\MOVIES folder.

Let's draw the cyclic Tyr-Ala-Trp. Again we will find **Clean Structure**  useful.



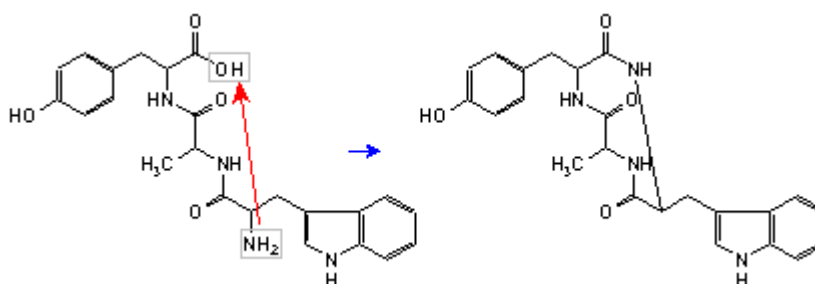
1. Make sure you are in the Structure mode.
2. In the **Template Window** that can be displayed with the **Open Template Window**  button, switch to the **Amino Acids** tab.
3. From the set of amino acids, click **Tyrosine** and click in the workspace to copy the structure.

4. From the **Table of Radicals** , choose sequentially **Alanine**  and then **Tryptophan**  and attach the corresponding radicals as indicated:

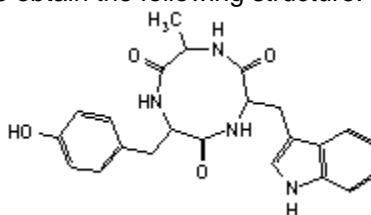


**Tip** You can flip the template shadow before placing it in the workspace by pressing TAB.

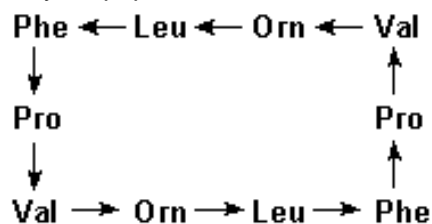
5. Right-click to quickly switch to the **Select/Move**  tool and drag the NH<sub>2</sub> group to the OH group as shown:



6. Click **Clean Structure**  to obtain the following structure:



⚠ Try to draw any other cyclic peptide, for instance Gramicidine S:



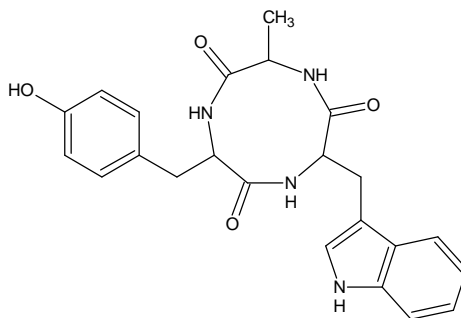
## 4.3 SMILES Notations

ACD/ChemSketch can convert SMILES (Simplified Molecular Input Line Entry Specification) strings to structures, and convert structures to SMILES

### 4.3.1 Generating SMILES Notations

Now we will try to create a SMILES string for the cyclic peptide drawn in Section 4.2.2.

1. On the **Tools** menu, point to **Generate**, and then choose **SMILES Notation**. The generated string appears right below the structure:



```
Oc1ccc(cc1)CC2NC(=O)C(C)NC(=O)C(NC2=O)C\C4=C\Nc3ccccc34
```

2. You can now copy the text string by selecting it and pressing CTRL+C to copy it to the Windows clipboard. Then paste it into any external text editor as text using the menu command or CTRL+V.

**Note** If you have several structures drawn on one page and you want to generate the SMILES string for all of them, you do not have to select them all—just leave them all unselected and repeat step 1. The SMILES notation appears for all the drawn structures as one string where each notation is separated by a point.

### 4.3.2 Generating Structures from SMILES Notations

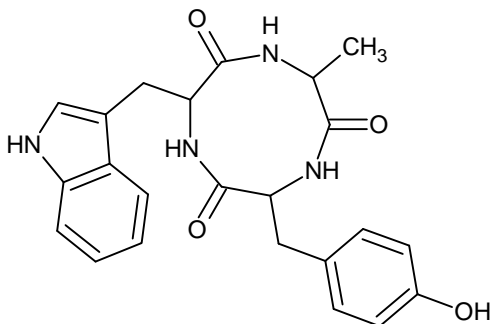
Now we will try the inverse task—generation of the structure from the SMILES string. At first we will generate the structure from the notation created in the previous section.

1. Select the text string created in the previous section:

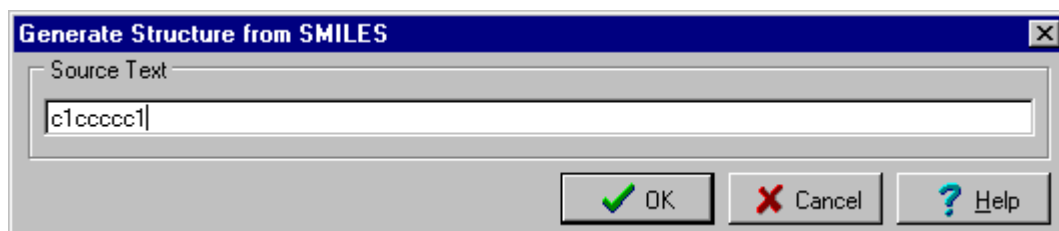
```
■ O c1 ccc(cc1)CC2NC(=O)C(C)NC(=O)C(NC2=O)C\C4=C\Nc3ccccc34 ■
```

2. On the **Tools** menu, point to **Generate**, and then choose **Structure from SMILES**. The generated structure is placed below the text string. As you can see, it is the same structure from which the SMILES notation was generated in the previous section:

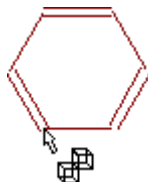
Oc1ccc(cc1)CC2NC(=O)C(C)NC(=O)C(NC2=O)C\C4=C\Nc3ccccc34





3. If you do not have the text string inserted into the workspace or it is not selected, selecting the **Structure from SMILES** command displays the following dialog box where you can type the string manually:



4. Click **OK**. The generated structure is attached to the cursor as a shadow:



5. Click in the workspace to place the structure.
6. On the General toolbar, click **Save File** , then click **New Page** .

## 4.4 InChI Notations

ACD/ChemSketch can convert InChI (IUPAC International Chemical Identifier) notations to structures, and convert structures to InChI strings.

InChI procedures were developed under IUPAC project. The technical development was carried out primarily at the US National Institute of Standards and Technology (NIST). More information about InChI is available on the IUPAC website at:

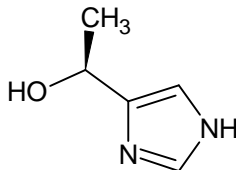
[www.iupac.org/inchi](http://www.iupac.org/inchi)



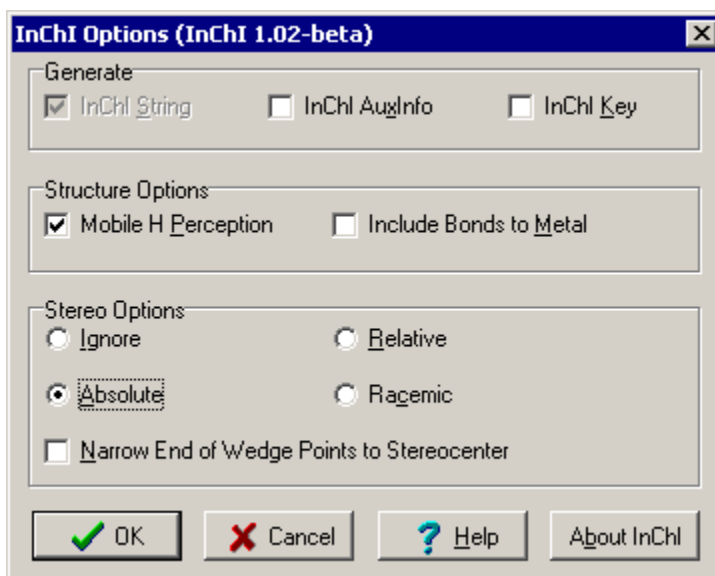
### 4.4.1 Generating InChI Notations

Now we will try to create an InChI string for (1S)-1-(1H-imidazol-4-yl)ethanol.

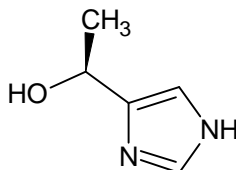
- Using the obtained skills, draw the following structure:



- On the **Tools** menu, point to **Generate**, and then choose **InChI Options**. In the dialog box that appears, specify options as shown and click **OK**:



- On the **Tools** menu, point to **Generate**, and then choose **InChI for Structure**. The generated string appears right below the structure:



InChI=1/C5H8N2O/c1-4(8)5-2-6-3-7-5/h2-4,8H,1H3,(H,6,7)/t4-/m0/s1

**Note** You can now copy the text string by selecting it and pressing CTRL+C to copy it to the Windows clipboard. Then paste it into any external text editor as text using the menu command or CTRL+V.

- Repeat the generation of the InChI string for the current structure but with the different options; in the **InChI Options** dialog box, clear the **Mobile H Perception** option and select **Ignore** under **Stereo Options**. The following InChI notation appears in this case:

InChI=1/C5H8N2O/c1-4(8)5-2-6-3-7-5/h2-4,8H,1H3,(H,6,7)/f/h6H

### 4.4.2 Generating Structures from InChI Notations

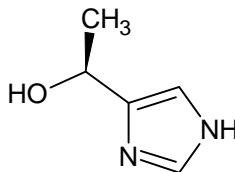
Now we will try the inverse task—generation of the structure from the InChI string. We will generate the structure from the notations created in the previous section.

1. Select the text string that was created first in the previous section:

```
InChI=1/C5H8N2O/c1-4(8)5-2-6-3-7-5/h2-4,8H,1H3,(H,6,7)/t4-/m0/s1
```

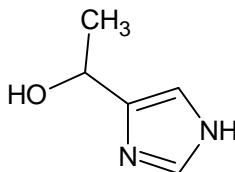
2. On the **Tools** menu, point to **Generate**, and then choose **Structure from InChI**. The generated structure is placed below the text string. As you can see, it is the same structure from which the InChI notation was generated in the previous section:

InChI=1/C5H8N2O/c1-4(8)5-2-6-3-7-5/h2-4,8H,1H3,(H,6,7)/t4-/m0/s1



3. Now select the second InChI string and choose the **Structure from InChI** command again. You can see that the stereoisomerism is not reflected:

InChI=1/C5H8N2O/c1-4(8)5-2-6-3-7-5/h2-4,8H,1H3,(H,6,7)/f/h6H



## 4.5 3D-Optimization

This section explains how to create structures that have “realistic” angles and bond lengths. There is no need to explain how difficult it is to draw such structures proportionally. The 3D-Optimization and 3D Rotation options will help you to quickly cope with this task. These options make it possible to create complex structures in ACD/ChemSketch with ease.



### 4.5.1 Creating Structure of Bicyclo[2.2.2]octane




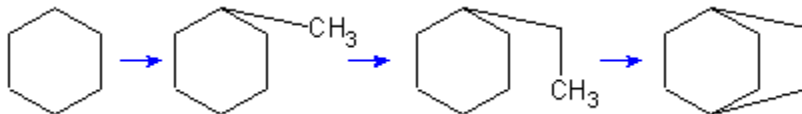
This section is based on the movie **bicyc.exe** which can be downloaded from our Web site or found in the \\MOVIES folder.







1. From the **Options** menu, choose **Preferences**, and, in the dialog box that appears, switch to the **Structure** tab.
2. In the **3D Optimization** area, clear the **Add Hydrogens** check box and click **OK**.


3. On the Reference toolbar or from the **Table of Radicals** , choose **Cyclohexane** . Click in the workspace to place a cyclohexane ring.

4. Click **Draw Normal**  and draw the hydrocarbon bridge by dragging as shown in the following scheme:




5. Click **3D Optimization**  to obtain a 3D model of the drawn structure.

**Note** If there is more than one structure in the workspace you should select the structure you want to optimize in 3D using any of the selection tools (**Select/Move** , **Select/Rotate/Resize** , or **3D Rotation**  tools).

6. If the Switch to **3D Rotation mode** check box in the **Structure** tab of the **Preferences** dialog box (**Options** menu) is selected, you will be automatically switched to 3D Rotation mode after the 3D Optimization is completed. If you are not, click **3D Rotation** . Point to any atom or bond on the structure and drag over the workspace to rotate the structure until it is placed as shown:



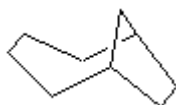
**Note** From the **Options** menu, choose **Preferences**, and then click on the **Structure** tab of the dialog box. You can choose whether the background bond should be broken or not by selecting or clearing the **Enable** check box in the **Bonds Intersections** area.

You can change the position of intersecting bonds by applying the **Bring Bond to Front** (CTRL+F) or **Send Bond to Back** (CTRL+K) commands (**Tools** menu) to the selected bond. You can also bring the background bond to the front by clicking it with the **Change Position**  tool active while holding down SHIFT.

Try to draw the following structures on your own using the above technique



Bicyclo[2.2.1]heptane



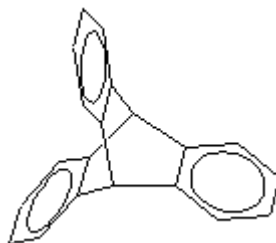
Bicyclo[4.2.1]nonane

7. On the General toolbar, click **Save File** , then click **New Page** .




## 4.5.2 Creating the Structure of Triptycene

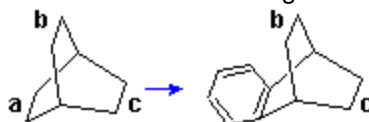


This section is based on the movie **triptyc.exe** which can be downloaded from our Web site or found in the \\MOVIES folder.

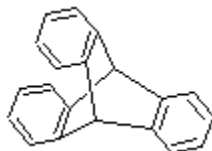






Make sure you are in the Structure mode.

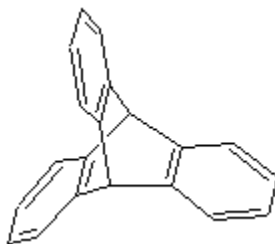
1. Draw the structure of *bicyclo[2.2.2]octane* as described above or, on the Structure toolbar, click **Template Window** , then click the **Bicyclics** **Bicyclics** tab or select the *bicyclics* in the list of templates above, and select the appropriate structure. Click in the workspace to paste it.
2. On the **Reference** toolbar or from the **Table of Radicals** , choose **Benzene** .
3. Point to the bond **a** and click to attach the benzene ring to this bond:




4. Repeat steps 2–3 for bonds **b** and **c** to obtain the following structure:

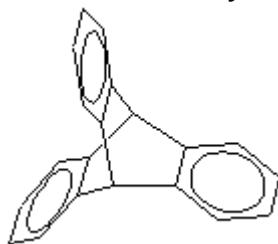


5. If there is more than one structure in the workspace, select the structure you want to 3D-optimize using any of the selection tools (**Select/Move** , **Select/Rotate/Resize** , or **3D Rotation**  tools).
6. Click **3D Optimization**  to obtain a 3D-model of the drawn structure:



7. If the **Switch to 3D-Rotation Mode** check box in the **Preferences** dialog box (**Structure** tab) is selected, the program will automatically switch to the 3D Rotation mode after the 3D-optimization is completed, if it does not, click **3D Rotation** . Point to any atom or bond of the structure and drag over the workspace to obtain the projection you want.

8. From the **Tools** menu, choose **Show Aromaticity** to show the aromatic rings:



9. On the General toolbar, click **Save File** , then click **New Page** .




### 4.5.3 Creating the Structure of Cubane

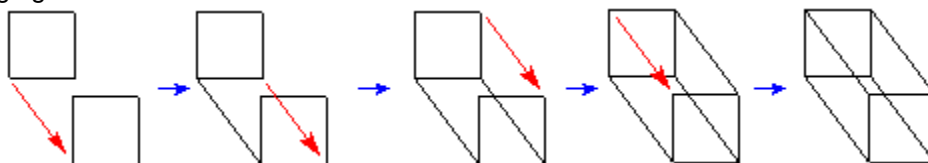




This section is based on the movie **Pr\_cub.exe** which can be downloaded from our Web site or found in the \\MOVIES folder.

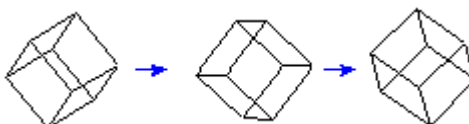


Make sure you are in the Structure mode.


- On the **Reference** toolbar or from the **Table of Radicals** , choose **Cyclobutane** . Click twice in the workspace to place two 4-membered rings one under another.
- Click **Draw Normal**  and connect the corners of the cyclobutane structures with bonds by dragging from one atom to another as shown:



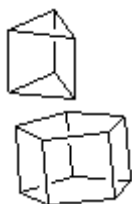
- Click **3D Optimization**  to obtain the 3D model of the drawn structure.
- Click **3D Rotation**  if it is not already selected.
- Point to any atom or bond on the structure and drag over the workspace to obtain the projection you want:



**Note** From the **Options** menu, choose **Preferences** and switch to the **Structure** tab of the dialog box. You can choose whether the background bond should be broken or not by selecting or clearing the **Enable** check box in the **Bonds Intersections** area.

You can change the position of intersecting bonds by applying the **Bring Bond to Front** (CTRL+F) or **Send Bond to Back** (CTRL+K) commands (**Tools** menu) to the selected bond. You can also bring the background bond to the front by holding down SHIFT and clicking it with the **Change Position**  tool active.

! Try to draw the following structures on your own using the above technique



Prismane

Hexacyclo[4.2.0.0<sup>2,5</sup>.0<sup>3,9</sup>.0<sup>4,8</sup>.0<sup>7,10</sup>]decane

6. On the General toolbar, click **Save File** , then click **New Page** .



#### 4.5.4 Creating the Structure of Dodecahedrane ([5]Fullerene-C<sub>20</sub>)

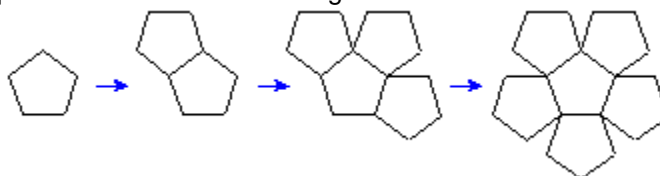



This section is based on the movie **fuller.exe** which can be downloaded from our Web site or found in the \\MOVIES folder.

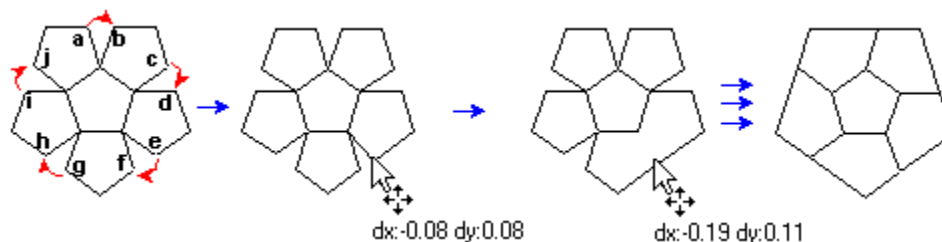
**Error! Objects cannot be created from editing field codes.**


Make sure you are in the Structure mode.

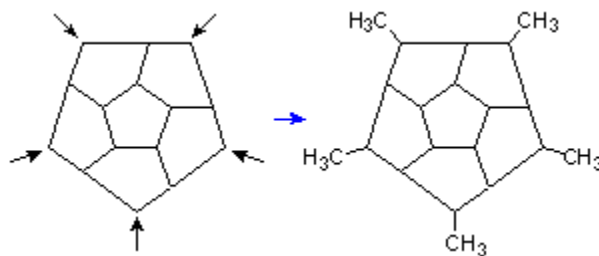
- On the Reference toolbar or from the **Table of Radicals** , choose **Cyclopentane** . Click in the workspace to place a cyclopentane ring.
- Sequentially point to each bond of the ring and click to attach five other rings:



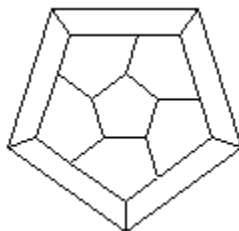
- Right-click to quickly switch to the **Select/Move**  tool.
- Move by dragging atoms **a, c, e, g, i** to atoms **b, d, f, h, j** accordingly as shown in the following scheme to merge them:





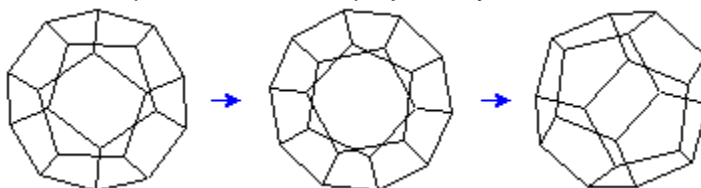
- On the Atoms toolbar, click **Carbon** , and click directly the points indicated by arrows to add more atoms and bonds:




6. Connect the adjacent methyl groups with single bonds by dragging from one terminal atom to another to obtain the following structure:



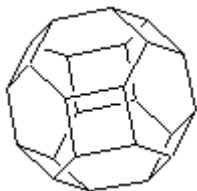
7. On the Structure toolbar, click **3D Optimization**  to obtain the 3D model of the drawn structure.
8. On the Structure toolbar, click **3D Rotation** . Point to any atom or bond on the structure and drag over the workspace to obtain the projection you want.



**Note** From the **Options** menu, choose **Preferences** and switch to the **Structure** tab of the dialog box. You can choose whether the background bond should be broken or not by selecting or clearing the **Enable** check box in the **Bonds Intersections** area.

You can change the position of the bonds of interest by applying the **Bring Bond to Front** (CTRL+F) or **Send Bond to Back** (CTRL+K) commands (**Tools** menu) to the selected bond. You can also bring the background bond to the front by holding down SHIFT and clicking it with the **Change Position**  tool active.

Try to draw the following structures using the technique described above

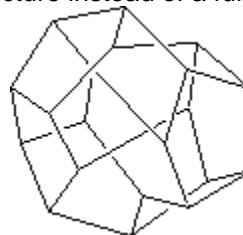





[4,6]Fullerene-C<sub>24</sub>



[5,6]Fullerene-C<sub>24</sub>

**Tip** If the optimization produces a “Moebius” structure instead of a fullerene-type structure



the optimization has converged to an unusual value. Click **Undo**  to return to your pre-optimized structure. Then, click **Clean Structure**  or, using the **Select/Move**  tool, move some of the atoms slightly and optimize again.

9. On the General toolbar, click **Save File** , then click **New Page** .

## 4.6 Drawing, Labeling, and Mapping Reactions

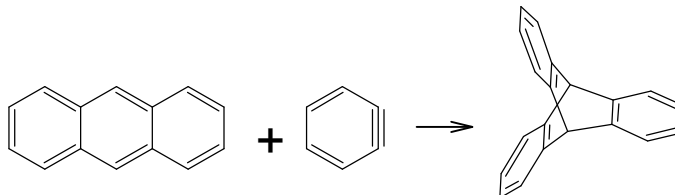
This section explains how to draw reactions and complex chemical schemes with manual or automatic mapping.



### 4.6.1 Drawing a Reaction Scheme



This section is based on the movie **reaction.exe** which can be downloaded from our Web site or found in the \\MOVIES folder.

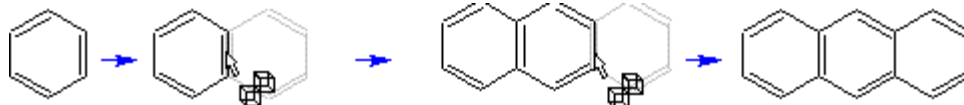
In this section, we will draw the following reaction scheme:



1. From the **Table of Radicals** , choose **Benzene**  (if you have recently used this template, you can find it on the **Reference** toolbar).

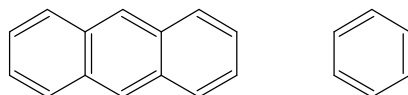



2. Press TAB to flip the template shadow and draw the following structure by clicking in the workspace several times:

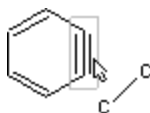


**Note** To draw a fused-ring structure, place the cursor directly over a ring bond and click.

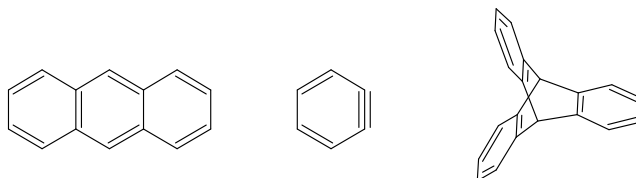
3. Press TAB to flip the shadow again and click beside the drawn structure to place a separate ring. Right-click to hide the template shadow.



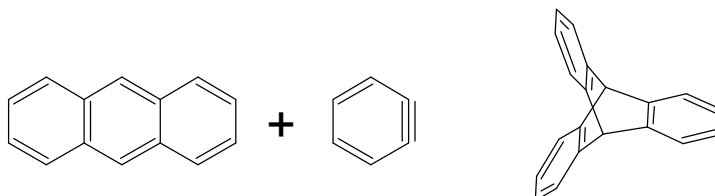
4. On the Structure toolbar, click **Draw Normal** , and then click the bond of the ring to make it triple:




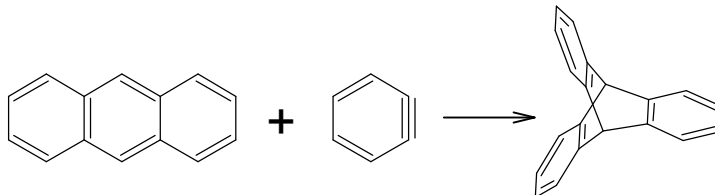
5. Draw the structure of Triptycene as described in Section 4.5.2 and place it beside the other drawn structures:




6. On the Structure toolbar, click **Reaction Plus** , and then place it between the first and the second structures by clicking:



7. Click **Reaction Arrow** , and click or drag to place it as well:





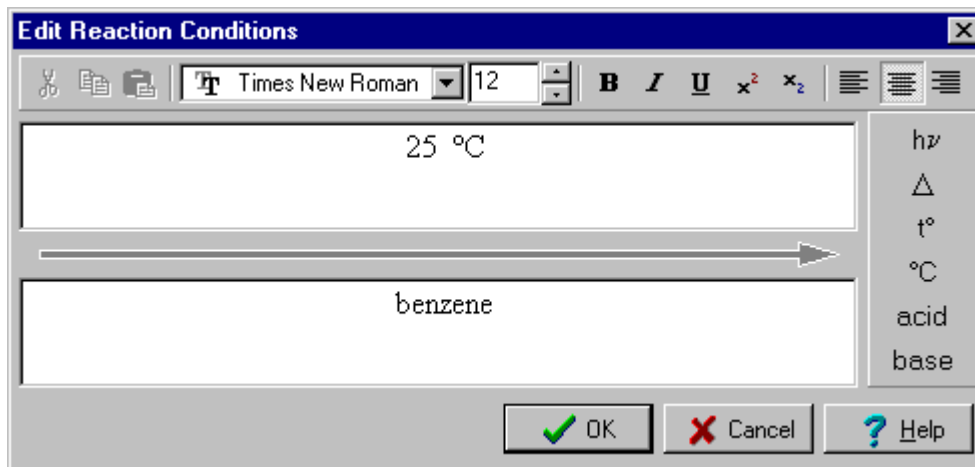
**Note** By clicking the bottom right triangle of the **Reaction Arrow**  button you can choose from a variety of arrows. Some arrows are treated as graphical objects, however, and cannot be exported properly.

8. To move the plus sign or the arrow, click **Select/Move** , point to the object, and then drag.

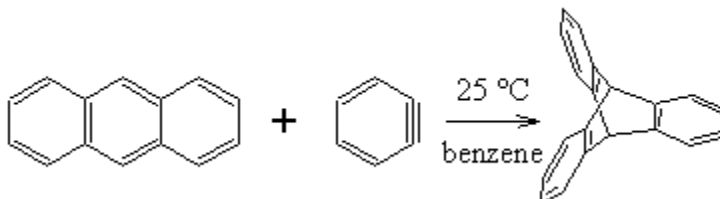
## 4.6.2 Labeling a Reaction

In this section, you will study how to add experimental conditions to a reaction scheme:

1. On the Structure toolbar, click **Reaction Arrow Labeling** .
2. Click the reaction arrow to display the **Edit Reaction Conditions** dialog box.
3. In the **Edit Reaction Conditions** dialog box, type "25" in the upper pane, and then click **C°**  on the right side of the dialog box.
4. Type *benzene* in the lower pane.



5. Click **OK** to close the dialog box. The reaction now looks like this:



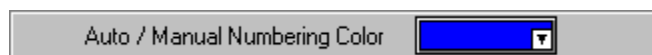
## 4.6.3 Mapping a Reaction

This tool allows you to map a drawn reaction either manually or automatically. To differentiate between the automatically generated and manually inserted numbers, select different colors for automatic and manual mapping.

1. From the **Options** menu, choose **Preferences** to display the **Preferences** dialog box.
2. Switch to the **Reaction** tab, and then select the red color in the **Manual Mapping Color** box:



3. Switch to the **Structure** tab, and then select the blue color in the **Auto/Manual Numbering Color** box.



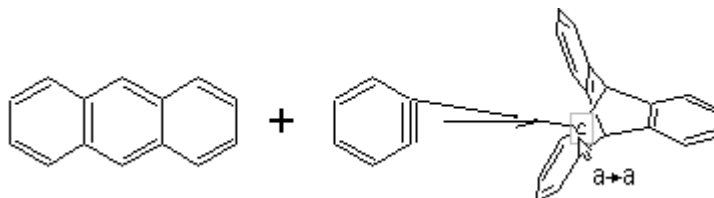
4. Click **OK**. Now, we can get down to mapping as it is.

5. On the Structure toolbar, click **Atom-Atom Map**  to display the **Map Tools** panel and enable the mapping mode:



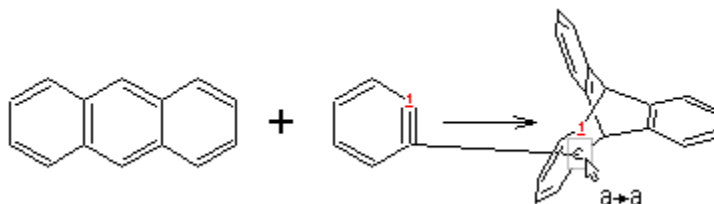
**Note** Note that the **Manual Mapping** mode is automatically enabled (the corresponding button is active).

6. Point to the atom in the reactant and drag to the corresponding atom in the product.



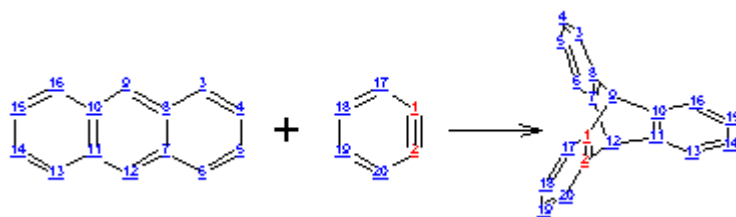
As you release the mouse button, **1** appears on the reaction scheme denoting manually mapped atoms.

7. Point to the next atom and drag again to its counterpart in the product:



As you release the mouse button, **2** appears near the reactant atom and near its counterpart on the product.

8. Now, on the **Map Tools** panel, click **Auto Mapping** . All other atoms are automatically assigned to each other:

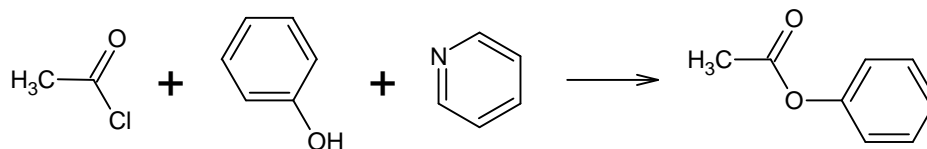


**Note** The mapped atoms are only visible when the **Map Tools** panel is displayed.


9. On the General toolbar, click **Save File** , then click **New Page** .

#### 4.6.4 Calculating Reaction Data—Commercial version only!

1. Using the acquirements (see Section 4.6.1), draw the following reaction:



Reactant	Formula	FW	K	n	C	m	V	d	Yield
1	C <sub>2</sub> H <sub>3</sub> ClO	78.4976	1	1.1 mol	-	86.3 g	78.5 mL	1.1 g/mL	-
2	C <sub>6</sub> H <sub>6</sub> O	94.1112	1	-	-	-	-	-	-
3	C <sub>5</sub> H <sub>5</sub> N	79.0999	1	-	-	-	-	-	-
Product									
1	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	136.1479	1	-	-	-	-	-	-

2. On the Structure toolbar, click **Reaction Calculator** , and then click the reaction arrow. The **Reaction Calculator** dialog box appears:

The screenshot shows the 'Reaction Calculator' dialog box with a 'Components' section containing a table identical to the one above. Below the table is a 'Show Total' checkbox which is checked. At the bottom are 'OK', 'Cancel', and 'Help' buttons.

- On the row that corresponds to acetyl chloride (C<sub>2</sub>H<sub>3</sub>ClO), double-click the Quantity cell (**n**) to select it.
- Type *0.11 mol*, and then press ENTER.
- To calculate the volume, you need to enter the density of the compound. Double-click the corresponding Density cell (**d**), and then type *1.1 g/mL*. After you press ENTER, the calculated value appears in the Volume cell (**V**).
- Similarly, insert the following values into the corresponding **Components** table cells: for phenol—*0.1 mol* for quantity (**n**), for pyridine—*0.11 mol* for quantity (**n**) and *0.983 g/mL* for density (**d**). All of the dependent data is automatically calculated.

7. Double-click the Mass cell (**m**) corresponding to the product and type 12.9 g.
8. Press ENTER. You will see that the yield is calculated and the **Based on** notation appears under **Yield** in the row corresponding to phenol:

React...	Formula	FW	K	n	C	m	V	d	Yield
1	C <sub>2</sub> H <sub>3</sub> ClO	78.4976	1	0.11 mol	-	8.63 g	7.85 mL	1.1 g/mL	-
2	C <sub>6</sub> H <sub>6</sub> O	94.1112	1	0.1 mol	-	9.41 g	-	-	Based on
3	C <sub>5</sub> H <sub>5</sub> N	79.0999	1	0.11 mol	-	8.7 g	8.85 mL	0.983 g/mL	-
Product									
1	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	136.1479	1	0.0947 mol	-	12.9 g	-	-	94.7 %
Total	-	-	-	0.32 mol	-	26.7 g	16.7 mL	-	-

9. Click **OK** to close the **Reaction Calculator** dialog box and paste the filled in **Components** table in the ChemSketch page.

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## 5. Advanced Drawing: Templates

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### 5.1 Objectives

This chapter brings you yet another step closer to advanced drawing expertise once you have mastered the powerful Template feature. You will learn:

- Some ways of template usage;
- How to apply the **Instant Template** tool to drawing the structures containing repetitive fragments;
- More ways of using the Table of Radicals;
- How to use the Template window for drawing DNA structures and complex biomolecular structures; and
- How to create your own templates.

### 5.2 Overview

ACD/ChemSketch includes the following three template tools for drawing structures:

- Table of Radicals 
- Instant Template 
- Template Window 

While the binding point of any template in the **Table of Radicals** is fixed (invariable), the Template window and the **Instant Template** tool allow you to specify any atom or bond to be the binding point simply by clicking it directly. However, no matter what the source of template is, the principles of joining are the same. There are several ways of joining the template to a drawn structure:

- By fusing the bonds of the structure and template: point to the bond so that the corresponding bonds of the structure and the template shadow are fused and then click.
- By attaching the template to the structure: point to the corresponding atom on the structure so that the connecting bond appears, and then click.
- By drawing a spiro connection between the template and the structure: point to the atom you want to be the binding point while holding down SHIFT, and then click.

**Note** You can flip the template shadow before fixing it by pressing TAB.

## 5.3 Table of Radicals

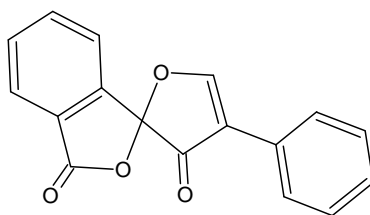
The Table of Radicals is a set of chemical radicals for structure drawing. Their names and, in some cases, abbreviations will help you to quickly translate “chemistry shorthand” into a meaningful structure.

### 5.3.1 Creating the Structure of Fluorescamine



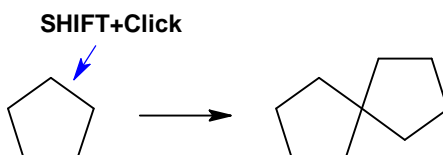
This section is based on the movie **fluor.exe** which can be downloaded from our Web site or found in the \\MOVIES folder.

We will draw the following structure using the templates taken from the Table of Radicals.

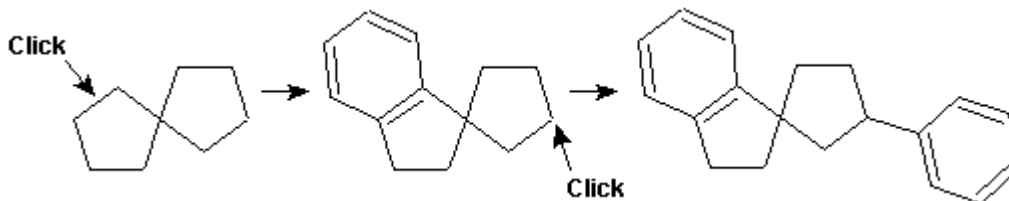




Make sure you are in the Structure mode.

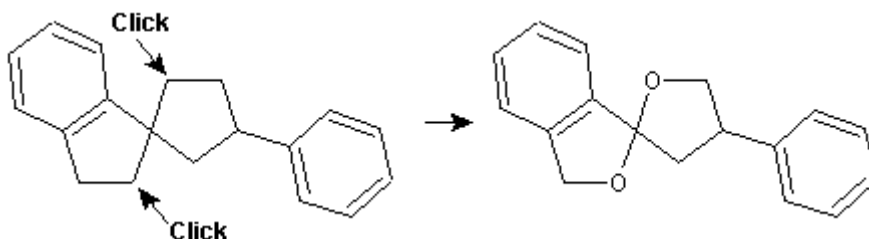
1. On the General toolbar, click **New Page** to open a new empty page.
2. On the Reference toolbar or from the **Table of Radicals** , choose **Cyclopentane** .
3. Click in the ChemSketch workspace to paste the ring.
4. Click the indicated atom while holding down SHIFT to obtain the spiro-connection with the second cyclopentane ring:



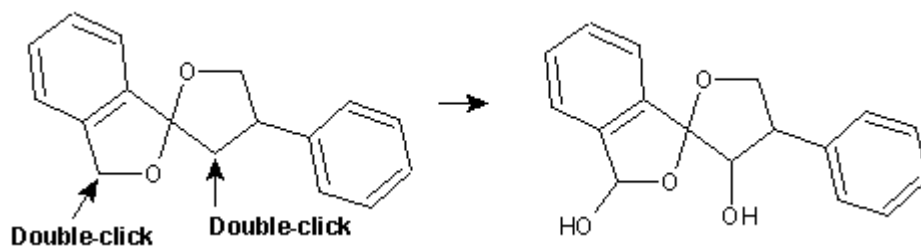
5. On the **Reference** toolbar or from the **Table of Radicals** , choose **Benzene** . First click the indicated bond to fuse the benzene ring and then click the indicated atom to connect the phenyl radical:



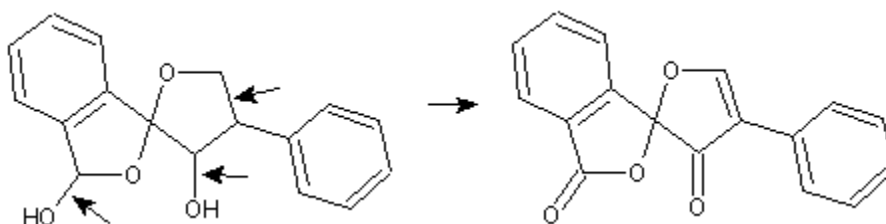
6. On the Atoms toolbar, click **Oxygen**  (note that the **Draw Normal** tool  is automatically enabled). Click the indicated atoms to replace them with oxygen atoms:



7. Right-click to quickly switch to the **Draw Continuous**  tool. Double-click the indicated atoms to attach the OH groups to them:




8. Click the indicated single bonds to replace them with double bonds:



9. On the General toolbar, click **Save File** , then click **New Page** .



## 5.4 Instant Template Tool

You might want to copy a molecular fragment that is not in the Table of Radicals. You can think of the **Instant Template** tool  as a “Paste” command. It is better than simple paste, however, because you can specify the point of attachment.




### 5.4.1 Creating the Structure of a Cyclic Oligomer

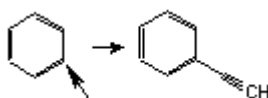


This section is based on the movie **oligomer.exe** which can be downloaded from our Web site or found in the \\MOVIES folder.

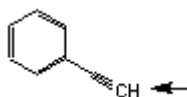
**Error! Objects cannot be created from editing field codes.**

Make sure you are in the Structure mode.

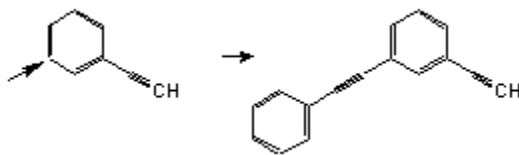
1. On the Reference toolbar or from the Table of Radicals () , choose **Benzene**  .  
Point to the upper middle part of the workspace and click to place a benzene ring.
2. From the Table of Radicals, choose **Ethynyl**  and click the atom indicated by the arrow to attach it to the ring:




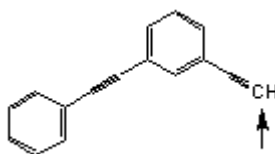
3. On the Structure toolbar, click **Instant Template**  and click the indicated atom to create an instant template:



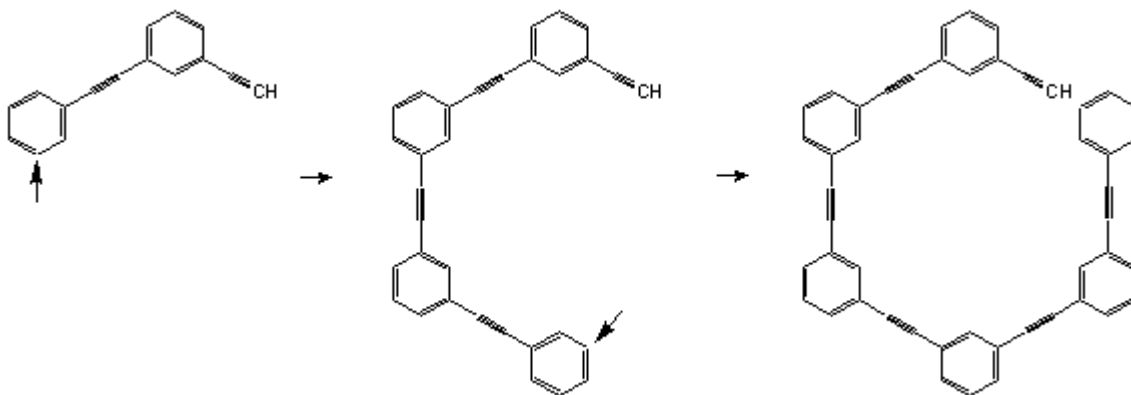
4. Click the atom indicated by the arrow to attach the template:




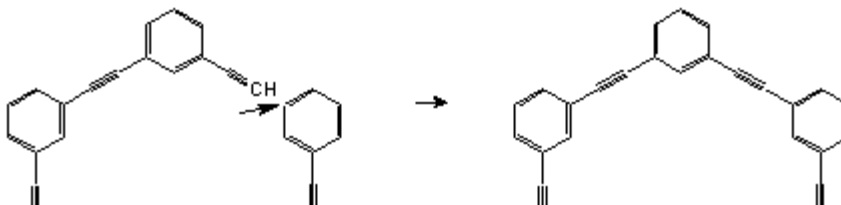
5. Click **Instant Template**  again and click the atom to create the template of the whole fragment:



6. Click the atoms to attach the template as shown. To hide the template shadow, right-click in the workspace after you finish drawing:



7. On the Structure toolbar, click **Draw Normal**  and click the indicated atom to complete the ring:



8. On the General toolbar, click **Save File** , then click **New Page** .

## 5.5 Template Window

The Template window feature is the most sophisticated of the three template features in ACD/ChemSketch because it allows you to organize and store structures or drawings that you might want to copy later.

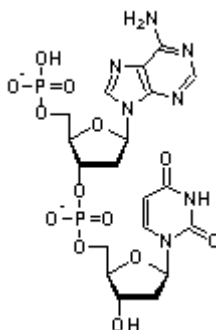


A brief tour of available ACD/ChemSketch Templates is given in the movie **templ\_st.exe** which can be downloaded from our Web site or found in the \\MOVIES folder.


### 5.5.1 Creating the Fragment of a DNA

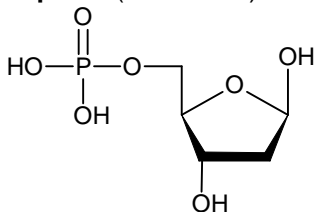


This section is based on the movie **dna\_st.exe** which can be downloaded from our Web site or found in the \\MOVIES folder.

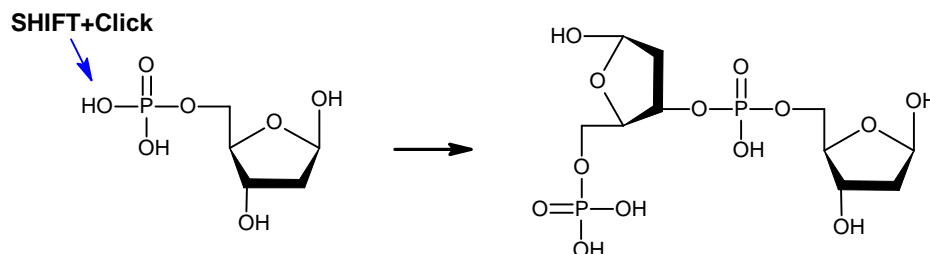


#### 5.5.1.1 Drawing the Chain of Deoxyribose-5-phosphate Fragments


1. On the General toolbar, click **Template Window** . On the **DNA/RNA Kit** tab, choose **2-Deoxyribose-5-phosphate** (chain form):

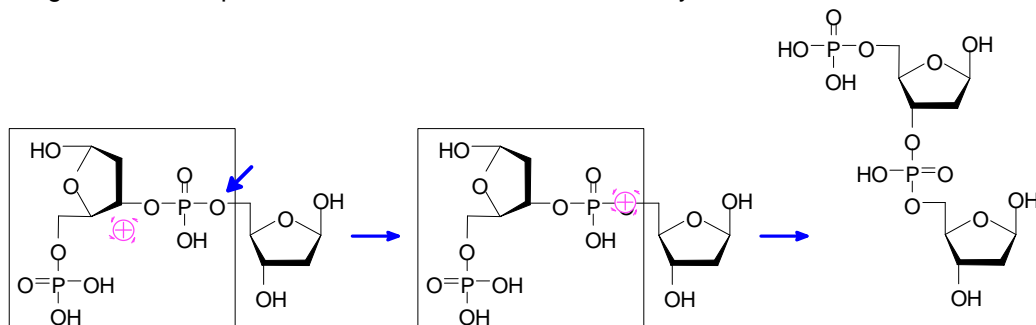


2. Click in the workspace to paste the chosen template.
3. Point to the indicated atom and holding down SHIFT click to attach the next 2-Deoxyribose-5-phosphate fragment:




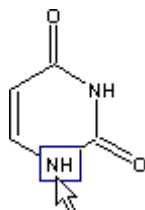
4. Click **Select/Rotate/Resize** .

5. Select the indicated part of structure by dragging the selection rectangle around it. Drag the action center  onto the oxygen atom indicated by arrow. Then, holding down SHIFT, drag the selected part of structure clockwise to rotate it by 90°:

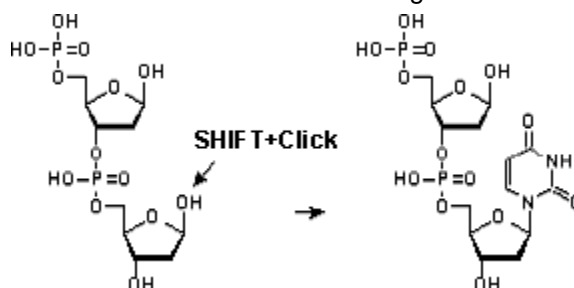


### 5.5.1.2 Adding the Bases

1. Open the **Template Window** . On the **DNA/RNA Kit** tab, choose the base you need by clicking the atom that will be the attachment point. For example, choose uracil, clicking the N atom shown so that this will be used as the attachment point:

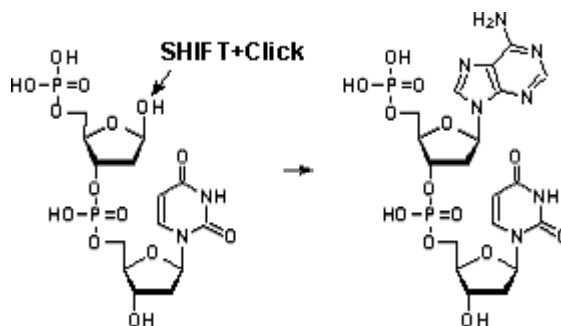


2. Point to the atom indicated below and click while holding down SHIFT:



**Tip** You can flip the template shadow before fixing it by pressing TAB.

3. Repeat steps 1 and 2 to add bases to other nucleotides such as adenine:



⚠ Now try to draw your own DNA or RNA fragment of any other length.

4. On the General toolbar, click **Save File** , then click **Close Document** .

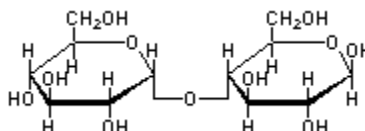
## 5.6 Drawing Complex Structures of Biomolecules


Here are some examples for creating complex structures of biomolecules using different ACD/ChemSketch tools.

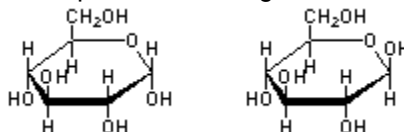
### 5.6.1 Creating the Structure of Beta-Maltose




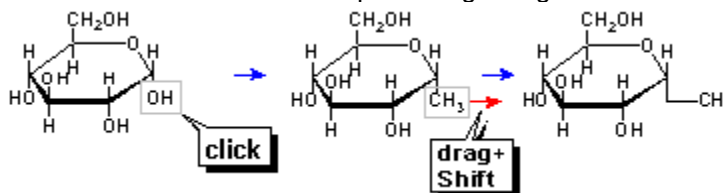
This section is based on the movie **maltose.exe** which can be downloaded from our Web site or found in the \\MOVIES folder.



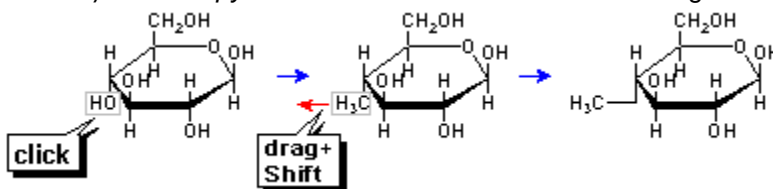
1. In the **Template Window** , switch to the **Sugars: alfa-D-Pyr** tab, and confirm that you are viewing the Haworth formulae page: 1(4) Haworth Formulae. If not, select it in the corresponding box.
2. Click  $\alpha$ -D-Glucopyranose to select it and click in the workspace to copy it.
3. Repeat steps 1–2, but this time select the beta-D-pyranose tab **Sugars: beta-D-Pyr** and choose  $\beta$ -D-Glucopyranose.
4. Click in the ChemSketch window to place it to the right of the first structure.



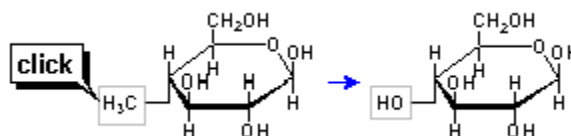
5. On the Atoms toolbar, click **Carbon** . Click the indicated atom in the  $\alpha$ -D-Glucopyranose structure to replace it with a CH<sub>3</sub> group and then drag from the CH<sub>3</sub> group to the right while holding down SHIFT to draw the bond at a perfect right angle:




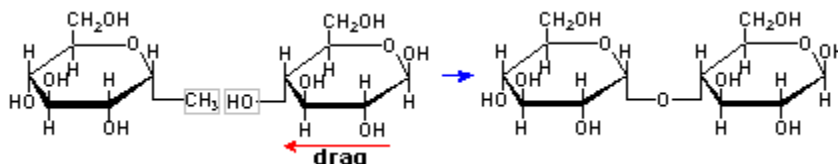
6. Repeat step 5 for the  $\beta$ -D-Glucopyranose structure to obtain the following structure:



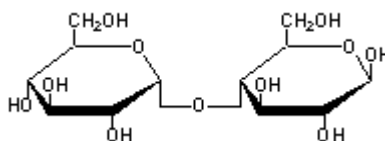
7. Click **Oxygen**  and click the indicated atom on the  $\beta$ -D-Glucopyranose structure:






8. On the Structure toolbar, click **Select/Move** . Click in the workspace adjacent to, but not touching, the  $\beta$ -D-Glucopyranose structure to select it. Point to any atom or bond of the selected structure and drag it to the left until the corresponding OH and CH<sub>3</sub> groups overlap each other:



9. If desired, hide single hydrogens in the selected structure; from the **Tools** menu, choose **Remove Explicit Hydrogens**:

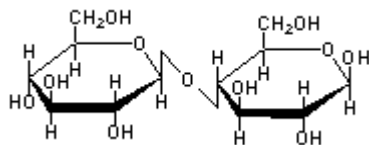


**Note** Though the carbon atoms bonded to central oxygen are hidden, they are still present. If the chemical meaning is important for your task (for example, in calculating the formula weight) you can remove these atoms in the following way.

With the **Select/Move**  tool active double-click the hidden atom. When the **Properties** panel appears; click the **Atom** tab, then click **Atom Symbol**  and from the **Value** drop-down list, choose **Empty** . Click **Apply**.

Alternatively, you can do this using the **Pseudo Atom**  tool.

! Try to draw the following structure on your own using the technique described above:



$\beta$ -Cellobiose

10. On the General toolbar, click **Save File** , then click **New Page** .

## 5.7 Defining a User Template

It is very easy to create a template out of a ChemSketch file. We are offering free templates, beyond those included with the ACD/ChemSketch installation package that can be downloaded from our Web site.<sup>2</sup> This is a templates exchange page, so if you have a set of structures or drawings that you think might be helpful to the ACD/ChemSketch community, consider sharing it!

To designate the structure(s) you have drawn as a template, we recommend that you:

1. Save the structures you have currently drawn to your examples folder, e.g., C:\EXAMPLES\ACD\MALTOSE.SK2.
2. From the **Templates** menu, choose **Save User Template**.
3. In the **Save User Template** dialog box, type the name for your template, such as Maltose, and specify the location of the file. Click **OK**.

**Note** You can enter any name for your document (e.g., for the document B\_D\_FUR.SK2 the following name—Sugars: beta-D-Furanose—would be the most appropriate).

Once your document is saved as a user template, the name you typed is automatically added to the list of templates in the Template window (from the **Templates** menu, choose **Template Window**).

**Note** You can create a user template from any document even if it is closed. From the **Templates** menu, choose **Template Organizer**. Click **New**, find the needed document, and assign a name to it.

4. Close the open document.

### 5.7.1 The Template Window Organizer

The **Template Window Organizer** is a very convenient way for managing template files: both those included with the software package, and those that you decide to create. It will just take you a minute to save your ACD/ChemSketch document as a template. Note that the only difference between the template file and a regular .SK2 file is the fact that the template file is assigned as a template in the Template Window Organizer. By saving files this way there are several advantages:

- Your .SK2 files scattered over different folders and disks will be gathered in one place (the Template Window Organizer).
- You can assign a name to the template that is more descriptive than the real file name is. This will better reflect the contents of the document and allow you to quickly find the document you need.

<sup>2</sup> Check first in the "Template" folder of the ACD/ChemSketch freeware for the desired template. If you don't find it there, go to [http://www.acdlabs.com/download/download\\_templates.html](http://www.acdlabs.com/download/download_templates.html).

- You can quickly find a document by previewing its contents in the Preview Area of the Template window.
- You can quickly open a selected document from the list by clicking **Open Document** in the Template Window Organizer.
- Up to 15 templates can be accessed through the Template window.

You can perform the following tasks with the user template:

- ⇒ Modify the template. From the Template List (**Template Organizer**) choose the needed template and click **Open Document**. Make changes as needed and save.
- ⇒ Copy any part of your template to the workspace (Structure or Draw mode) without opening the whole document. To do this, find your template in the Template List (Template window) and click the item to place it into the workspace.

### 5.7.2 The Template.cfg File

The key to management of the templates in ACD/ChemSketch is the file TEMPLATE.CFG. This file lets ACD/ChemSketch know that an .SK2 file is a template file rather than simply a user file. It can be opened and read with any text editor, although you will likely never need to do so. The Template window accesses TEMPLATE.CFG to let it know what files to display as templates. If an .SK2 file is not shown in the Template window, it will be added to TEMPLATE.CFG when you open .SK2 as a regular ACD/ChemSketch file and select the command to save as a user template.

If TEMPLATE.CFG is moved or lost, the Template window will not display any templates. If the TEMPLATE.CFG file is found (by Windows Explorer, for example, or the system "Find File" utility) it can be restored to the default directory or the user's private folder. If it cannot be found, it can be retrieved by reinstalling ACD/ChemSketch or by adding each template as described above.



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## 6. Calculating Macroscopic Properties

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### 6.1 Overview

In addition to the drawing capabilities, ACD/ ChemSketch offers predictions of numerous properties for your compounds.

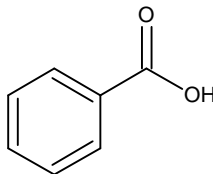
In this chapter, the simple means to calculate these properties is described.

### 6.2 Calculating Macroscopic Properties

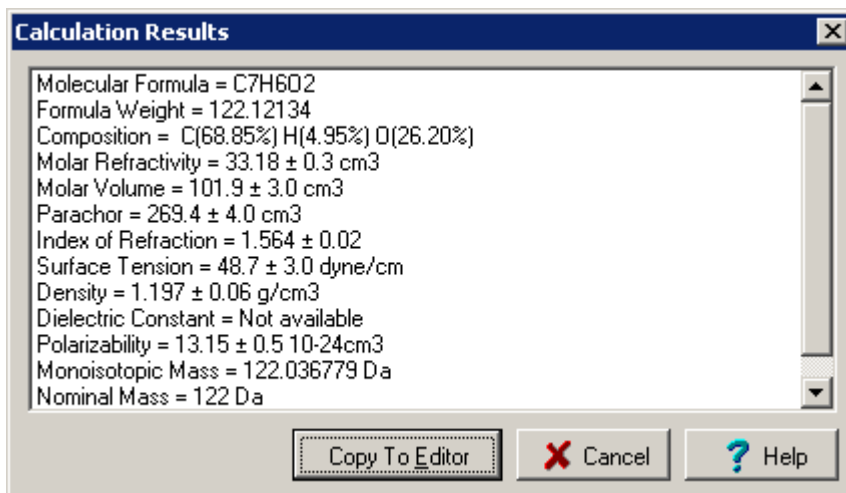
#### 6.2.1 Menu Command

To determine some or all of the available molecular properties, follow the steps:

1. When in Structure mode, draw a structure, for example, benzoic acid:



2. On the **Tools** menu, point to **Calculate**, and then choose **All Properties** or one of the available properties.
3. Once chosen, the calculated property is displayed in the **Calculation Results** dialog box. For example, choosing **All Properties** for benzoic acid will show the following dialog box:



- The result can be immediately pasted on the workspace if desired by clicking **Copy to Editor**. As the text is inserted, you are switched to the **Draw** mode that allows you to edit the text if necessary.

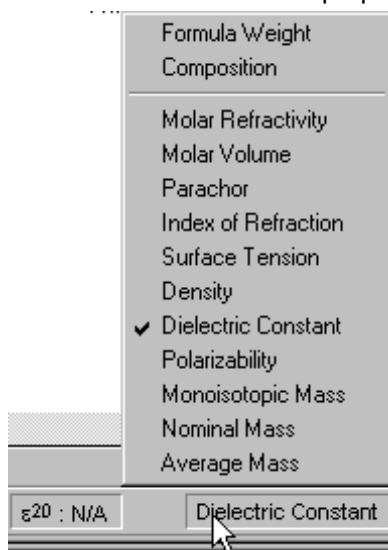
**Note** On the **Tools** menu, point to **Calculate**, and then choose **Select Properties to Calculate** to define a set of properties to be calculated. In the dialog box that appears, mark the properties and click **OK**. If you now choose **Selected Properties** only the selected properties will be calculated.

- Switch back to the **Structure** mode and save the document to CALC\_PROP.SK2.

## 6.2.2 Automatic Display on Status Bar

It is also possible to view the macroscopic property for the structure selected in the workspace directly on the status bar. Note that if no structure is selected in the workspace, the property is calculated for all the structures displayed; if there are no structures drawn, the field on the status bar is not available.


Click the field to the right on the status bar and choose the property desired.

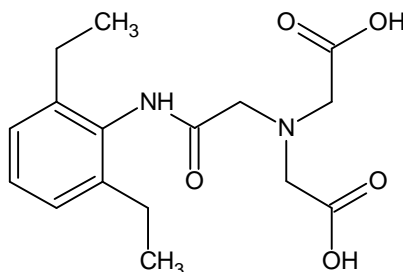



By default, this is set to formula weight. In the example shown, the dielectric constant,  $\epsilon^{20}$ , has been specified.

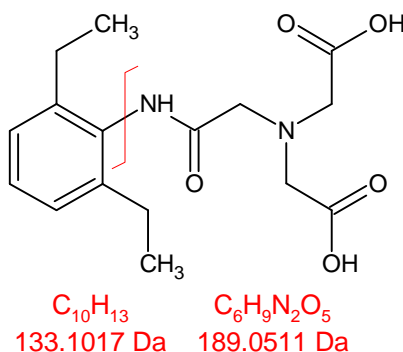
### 6.3 Calculating Monoisotopic Mass for a Fragment (MassSpec Scissors)

In this section, we'll calculate monoisotopic mass for a structural fragment:

1. On the General toolbar, click **New Page**  to open a new empty page.
2. Draw a structure, for example, the following one:



3. Select a bond to cut (it should be a non-cyclic one).
4. From the **Tools** menu, choose **MassSpec Scissors**, or, on the Structure toolbar, click the corresponding button . It will display monoisotopic mass underneath BOTH fragments in the workspace:



**Note** You can change the style of the separating line in the Draw mode: select the line, double click it, and, on the **Objects Panel**, change the style.

You can also see the nominal and average mass, using the **Calculate Macroscopic Properties** option (refer to Section 6.2).

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## 7. Special Function Keys


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### 7.1 Objectives

The ACD/ChemSketch is an extremely versatile molecular structure editor. For this reason, several ACD/Labs modules are now accessible as buttons from the ACD/ChemSketch interface. This chapter describes three special modules which can also be accessed from the ACD/ChemSketch interface. ACD/Tautomers and ACD/ Name Freeware are now included with both commercial and freeware versions of ACD/ChemSketch; ACD/Dictionary is also available but only with the commercial software.

### 7.2 Tautomers

For certain compounds, there is a mixture of two or more structurally distinct forms which exist in rapid equilibrium in solution. In most cases, tautomers result from a form of proton transfer. ACD/Tautomers is designed to generate the most reasonable tautomeric forms of drawn organic structures. It is available as the **Check Tautomeric Form** command through the **Tools** menu or as a button  on the Structure toolbar.

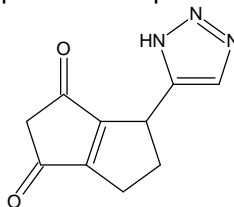
The possibility of the alternative tautomeric forms should always be carefully considered, if the drawn organic structure contains two or more double or triple bonds conjugated with or attached to oxygen, nitrogen, sulfur, or other heteroatoms. The current ACD/Tautomers algorithm provides only the suggested tautomeric forms, but not necessarily the correct forms. Consult other sources of information to make a final decision.



The ACD/Tautomers algorithm **does not** proceed with the following classes of chemical structures:

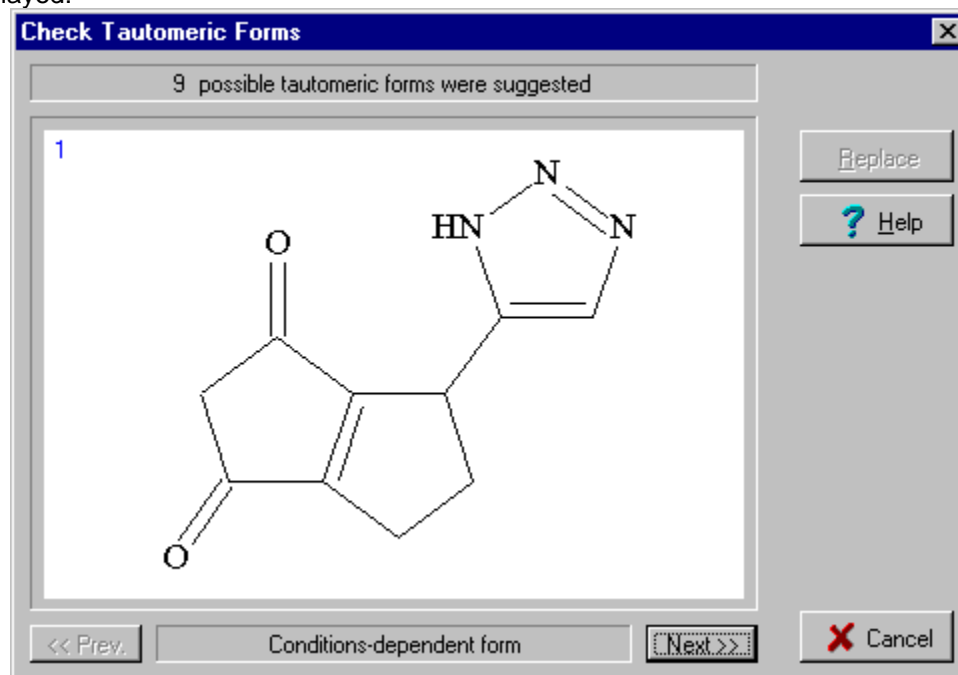
- Structures containing metal atoms;
- Structures containing charged atoms, other than the non-ionic derivatives of IV-valent nitrogen (+) bonded to oxygen (-);
- Structures containing elements in their non-typical valence;
- Structures with coordinating bonds; and
- Structures containing more than 255 atoms.

Now we are going to try this option on the illustrative example:

1. Using the technique described in the previous chapters draw the following structure:



2. Select the structure (use the **Select/Move**  tool), and, on the Structure toolbar, click **Check for Tautomeric Forms** . The program starts generating and checking tautomeric forms of the drawn structure and when the process is finished, the following dialog box is displayed:



3. Select the required tautomeric form using the **Next >>** or **<< Prev** buttons.  
 4. Click **Replace** to change the drawn structure for the currently selected one.

### 7.2.1 Examples

Here are a few “classic” types of tautomerism which you can try out with the Check Tautomeric Forms feature described above.

Tautomerism	Example
Keto-Enol	$\begin{array}{ccc} \text{H}_3\text{C}-\text{CH}_2-\text{C}(\text{H}_3)=\text{CH}-\text{CH}_2-\text{CH}_3 & \rightleftharpoons & \text{H}_3\text{C}-\text{CH}_2-\text{CH}(\text{H}_3)-\text{C}(=\text{O})-\text{CH}_2-\text{CH}_3 \\ & & \text{OH} \end{array}$
Phenol-keto	$\text{C}_6\text{H}_5\text{C}(\text{O})\text{H} \rightleftharpoons \text{C}_6\text{H}_5\text{OH}$
Heterocyclic ring	$\text{Pyridine} \rightleftharpoons \text{2-Hydroxypyridine}$

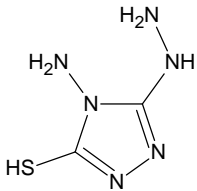
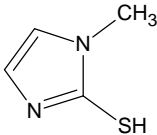
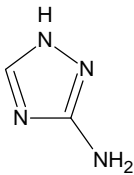
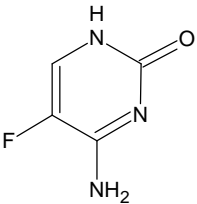
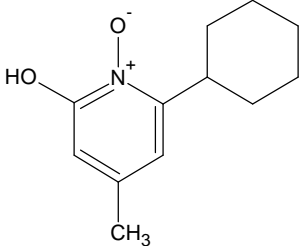
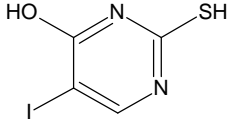
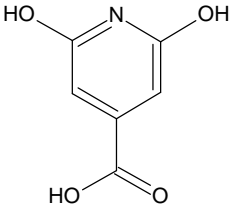
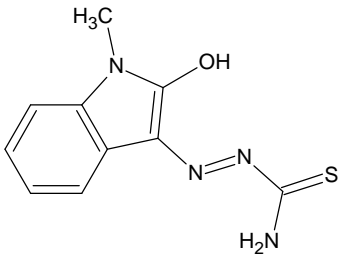
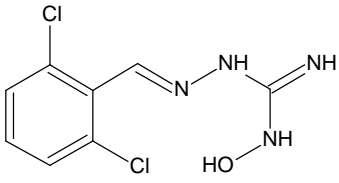
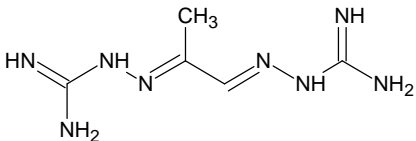
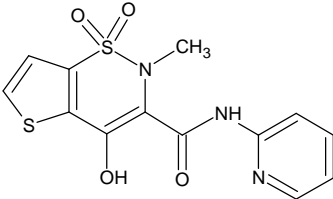
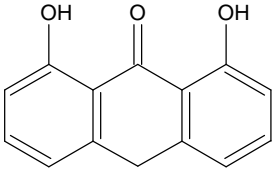
Tautomerism	Example
Nitro-acid form	
Nitroso-oxime	
Imine-Enamine	

## 7.2.2 Mistakes in the Chemical Literature

Chemical structures are often drawn as one tautomeric form, and other existing forms are simply ignored. Unfortunately, you can never be sure that a particular compound will be drawn the same way by another chemist. Therefore, the consideration of possible tautomeric forms is very important for structure search, data prediction, and interpretation.

All of the structures below have been taken from respected publications. Many have incorrect or ambiguous assignment of tautomeric forms under the experimental conditions described. With ACD/Tautomers, you no longer run the risk of overlooking a common tautomeric form for the compound you are trying to publish, interpret observed data for, or run ACD/Labs predictions on.

Questionable Structures from Various Publications		
Thioguanine (antineoplastic) 12 possible forms	6-Mercaptopurine (antineoplastic) 6 possible forms	Allopurinol (antiuric) (antiuric) 6 possible forms
Leucopurin >10 possible forms	Chlorzoxazone (skeletal muscle relaxant) 2 possible forms	Pemoline (CNS stimulant) 3 possible forms


Questionable Structures from Various Publications		
 <p>Purpald 4 possible forms</p>	 <p>Methimazole (antihyperthyroid) 2 possible forms</p>	 <p>Amitrole (herbicide) 5 possible forms</p>
 <p>Flucytosine (antifungal) 6 possible forms</p>	 <p>Ciclopirox (antifungal) 2 possible forms</p>	 <p>Iodothiouracil (thyroid inhibitor) 6 possible forms</p>
 <p>Citrazinic acid 2 possible forms</p>	 <p>Methisazone (antiviral) 2 possible forms</p>	 <p>Guanoxabenz (antihypertensive) 3 possible forms</p>
 <p>Mitoguazone (antineoplastic) &gt;10 possible forms</p>	 <p>Tenoxicam (anti-inflammatory, analgesic) 4 possible forms</p>	 <p>Anthralin (antipsoriatic) 2 possible forms</p>

## 7.3 Dictionary—Commercial version only!


ACD/Dictionary is an add-in module that is supplied with all the commercial copies of ACD/ChemSketch. It is immensely useful at finding “chemicals” by their common names.

ACD/Dictionary finds chemical structures according to their chemical name. It contains more than 125,000 systematic and non-systematic names and their corresponding molecular structures. The dictionary is searchable by both the full chemical name and name fragments.

ACD/Dictionary is covered in full in the *ACD/Dictionary User's Guide*, located in the ACD/Labs documentation folder, \\DOCS\\DICT.PDF.

**Note** If you have purchased ACD/ChemSketch, but do not see the **Dictionary** button  in the ChemSketch window when you are in the Structure mode, please verify that you have correctly entered TWO registration numbers at the time of installation—the one for ACD/ChemSketch (Main), and another for the ACD/Dictionary (Add-in).

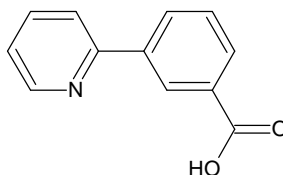
## 7.4 ACD/Name Freeware Add-on


Now it's possible to use ACD/Name Freeware Add-on right in the ACD/ChemSketch. This extra functionality is available as a button on the General toolbar: .

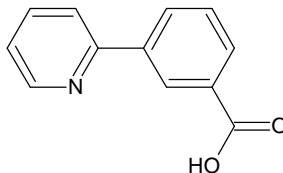
This tool is easy to use: draw the structure or structures to be named, click this button and the name for one structure or a mixture is inserted as a text string into the workspace.

Let's try naming some examples.

1. Using ChemSketch tools, draw the following structure:





2. If there is more than one structure drawn in the workspace, select the above structure only.
3. On the General toolbar, click **Generate Name for Structure**  or, on the **Tools** menu, point to **Generate**, and then choose **Name for Structure**. The name appears below the drawn structure:

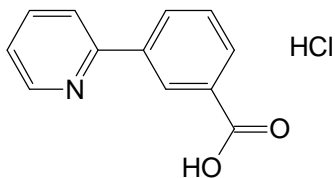


3-(2-pyridinyl)benzoic acid

**Note** The name generation preferences specified either in ACD/Name or any ACD/Labs Database program affect the result of the name generation in ACD/ChemSketch.



4. Move the name string down by dragging it.
5. On the Atoms toolbar, click **Chlorine**  and click once near the structure to draw HCl.
6. Select both structures and click **Generate Name for Structure**  again. This time the name for a mixture appears:



3-(2-pyridinyl)benzoic acid hydrochloride

### 7.4.1 Limitations of ACD/Name Freeware

ACD/Name Freeware has the following limitations:

- Structures to be named can contain no more than 50 atoms, including hydrogen.
- Structures can only contain the elements H, C, N, P, O, S, F, Cl, Br, I, Li, Na, and K in their common valences.
- Structures can contain no more than 3 cycles.
- The freeware version does not allow you to change the naming preferences. It uses the preferences that correspond to the most preferable IUPAC names.

**Note** For more information on ACD/Name, visit our Web site at [http://www.acdlabs.com/products/name\\_lab/name/](http://www.acdlabs.com/products/name_lab/name/)

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## 8. Searching for Structures— Commercial version only!

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### 8.1 Objectives

In this section, you will obtain some basic skills on how to perform searches for structures from ACD/ChemSketch environment.


In this section, you will learn how to:

- Perform searches for structure in the files on your computer;
- Customize the search options to suit your requirements;
- Set a mask for files to be searched through;
- View the search results.

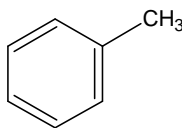
### 8.2 Searching for Structure


ACD/Name to Structure module allows you to search for drawn chemical structure(s) in a variety of files without opening them. As the structure is found, it can be viewed and placed either into the ChemSketch window or to the other applications.

#### 8.2.1 Which Files to Search Through?

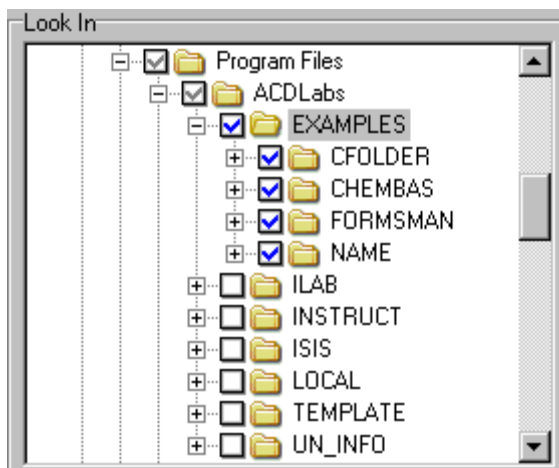
The **Search for Structure**  tool allows you to search for specific structures through the files of currently available formats.

1. On the General toolbar, click **New Page**  to switch to a new page.
2. Draw a structure of *toluene* or find it in ACD/Dictionary:

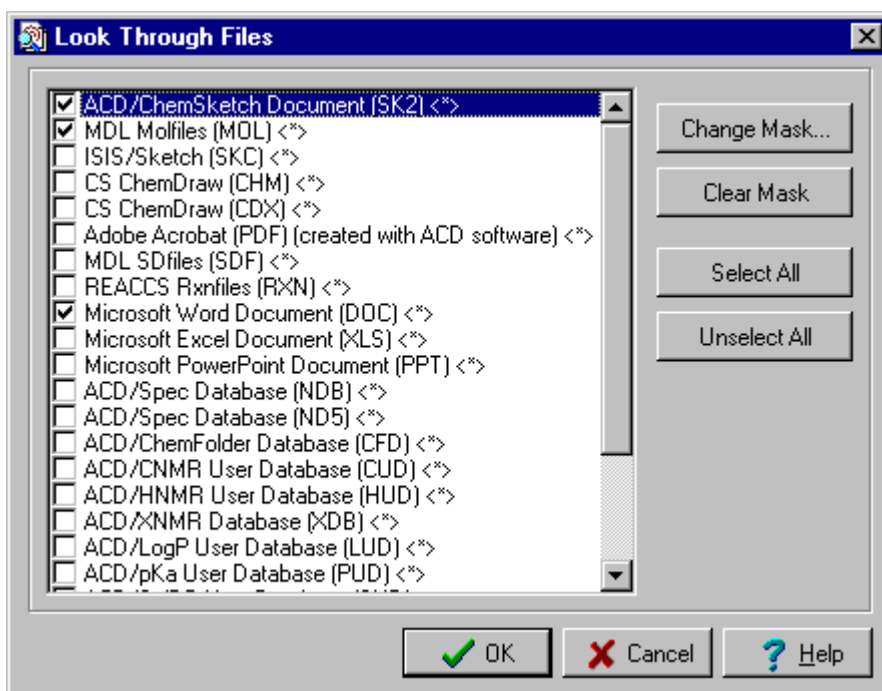


3. On the General toolbar, click **Search for Structure** . The **Search for Structure** dialog box containing the drawn structure in the **Search Pattern** box appears.

4. In the **Look In** box, select the folders and/or files to search through. For our example, find the ACD/Labs example folder and select it with all of the subfolders:



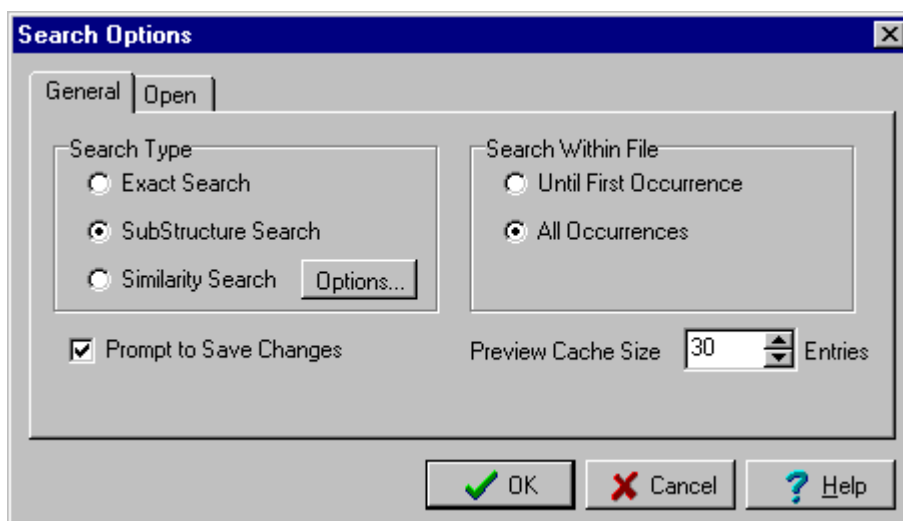
5. To set the formats of the files to search through, click **Browse** ... below the **Look In** box. The **Look Through Files** dialog box appears. Select the **ChemSketch Document**, **MDL Molfiles**, and **Microsoft Word Document** check boxes. Clear all the other check boxes.



**Tip** You can narrow the search by defining the file mask for any of the selected formats. Highlight the form and click **Change Mask** and in the dialog box that appears type a mask.

6. Click **OK** to apply your changes.

7. In the **Search for Structure** dialog box, click **Options** to customize the search options.

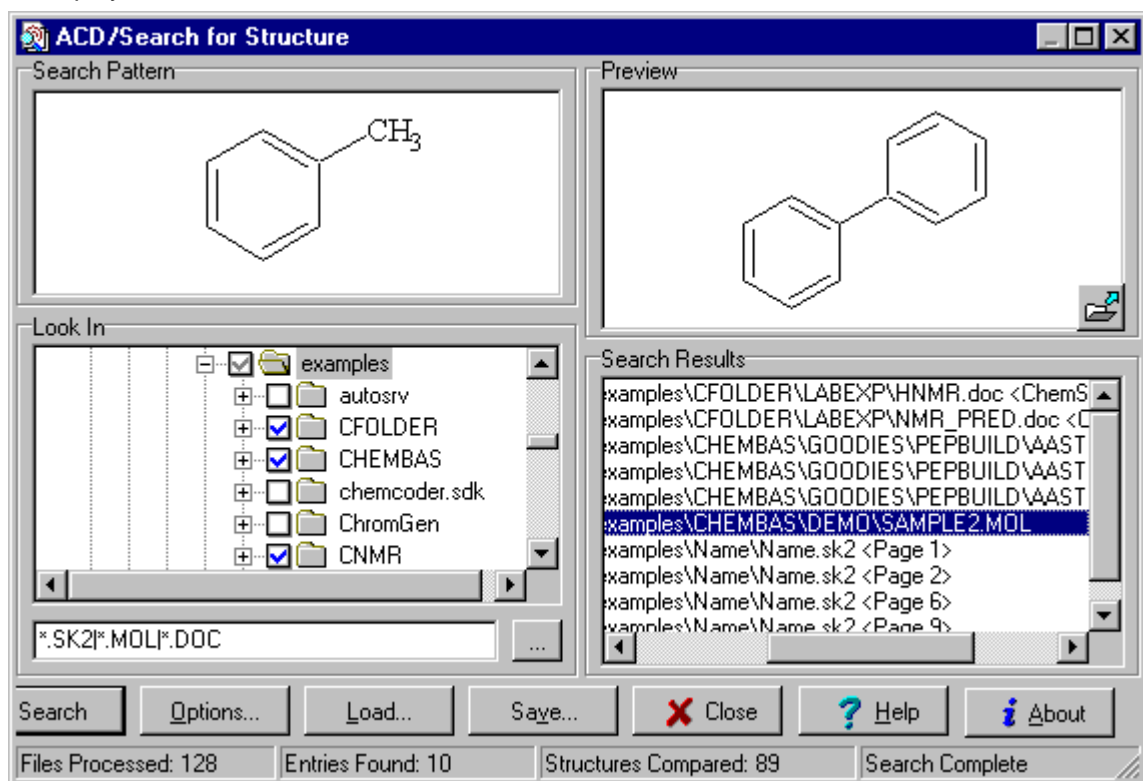


8. On the **General** tab, set the **Search Type** to **Substructure Search** and in the **Search Within File** box, choose **All Occurrences**.
9. Switch to the **Open** tab and if necessary define the applications to be used for opening the corresponding files.
10. Click **OK**.

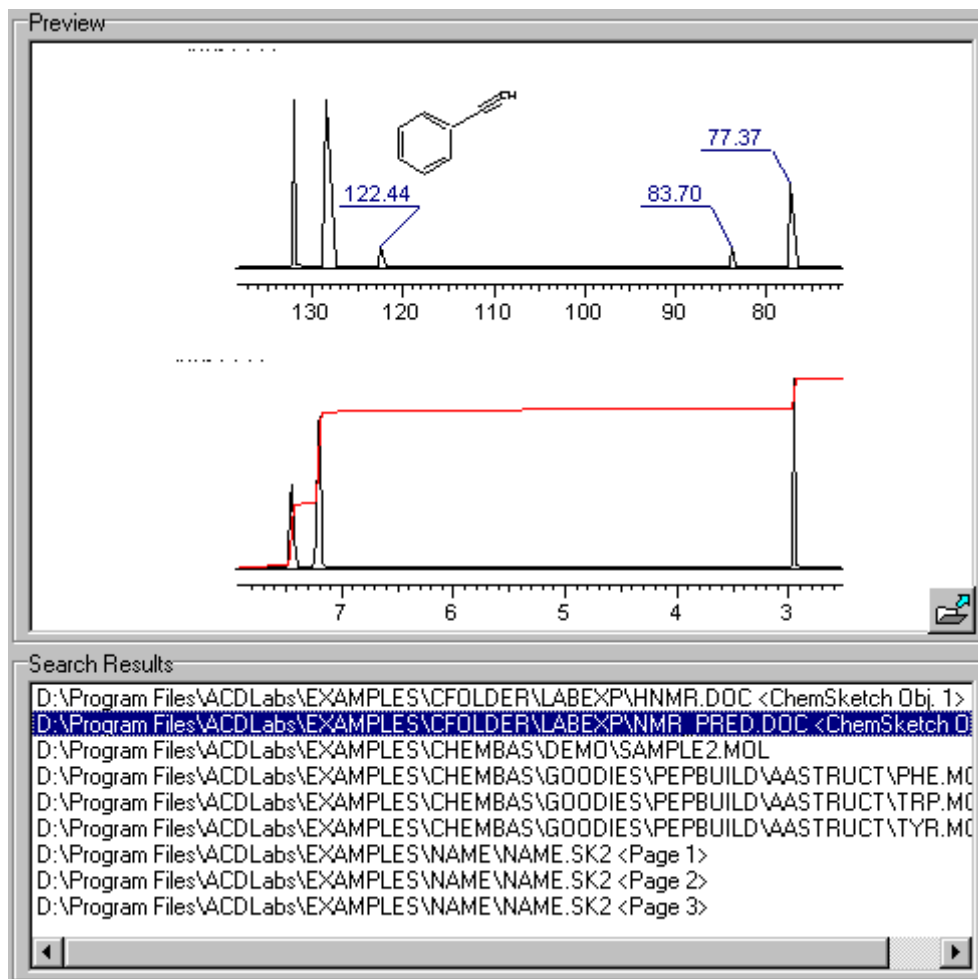
## 8.2.2 Considering Search Results


Now we can start search for the desired structure:

1. To start a search, click **Search**. As the search proceeds, the files where the query structure is found are displayed in the **Search Result** area.
2. To view the structure found by your query, click the list of found files. The structure is displayed in the **Preview** area.




3. If among the search results, there is a MS Word file (.DOC), clicking it in the list will display the OLE object that contains the query structure. For example:



4. To open the found structure or OLE object, click **Open**  in the **Preview** area.
5. To save the search results, as well as the query structure and folder settings, into an .SSF file, click **Save**.

**Note** If a found file is open in ACD/ChemSketch, a new page is created whose name fully corresponds to the path of the found file in the **Search Results** list. As the opening takes place, you do not leave the **Search for Structure** dialog box.

Therefore, each time you click **Open** , or double-click the same file highlighted in the **Search Results** list, a new page is opened in ACD/ChemSketch.

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## 9. Creating Graphical Objects

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### 9.1 Objectives

This chapter will familiarize you with the creation of graphical objects. Switch to the Draw mode before proceeding with any exercise in this chapter.

You will learn how to use Draw mode tools for creating the following objects:

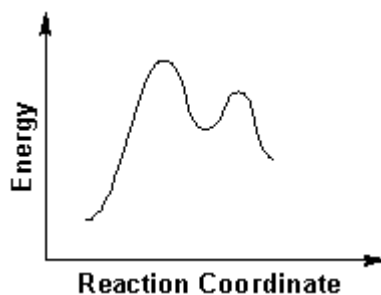
- A diagram of the energy of reaction
- Various types of orbitals
- Vacuum distillation apparatus
- A two-chain DNA strand
- Lipids and micelles
- Multipage layout posters

You will also learn how to output PDF files, a task that can be done for graphical or chemical objects.

### 9.2 Drawing the Energy of Reaction Diagram




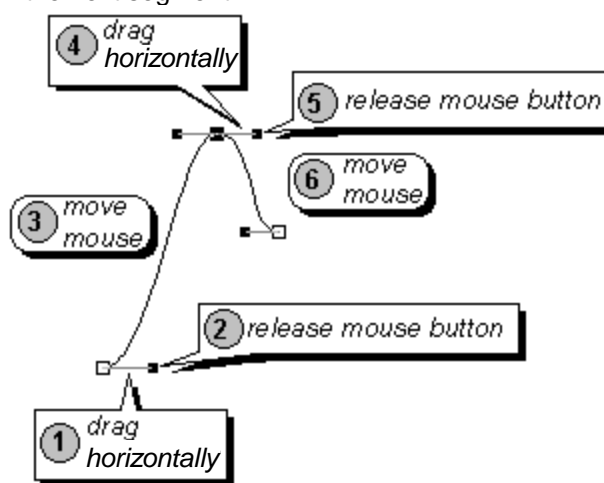
This section is based on the movie **diagram.exe** which can be downloaded from our Web site or found in the \\MOVIES folder.



### 9.2.1 Drawing a Curve

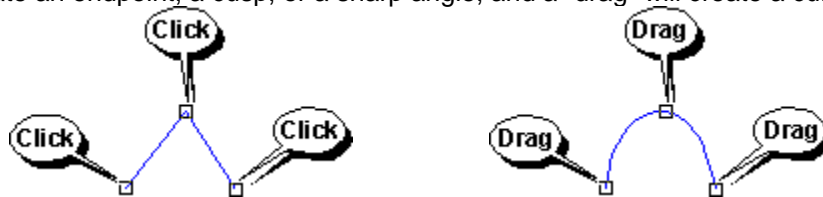
This section describes how to draw a curve:

1. Switch to the Draw mode by clicking **Draw** on the General toolbar.
2. Form the **File** menu, choose **New** to start a new document.
3. On the Drawing toolbar, click **Polyline** .
4. Drag horizontally to the right from the starting point of the curve to stretch the control line.
5. Release the mouse button.
6. Move the mouse up to draw the first segment of the curve.
7. Drag horizontally to the right to stretch the control lines. By changing the length of the control lines you can modify the curve segment.
8. Release the mouse button.
9. Move the mouse down to draw the next segment.




10. Repeat the above steps to draw the next two segments.
11. Right-click to finish drawing the curve.

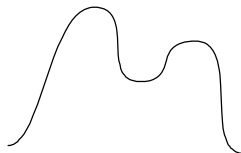
**Tip** When drawing with the **Polyline**  tool, it is helpful to remember that a “click” will create an endpoint, a cusp, or a sharp angle, and a “drag” will create a curve:







## 9.2.2 Modifying a Curve

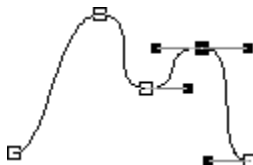
The first time you draw with the **Polyline**  tool you might have some trouble getting the curve to turn out the way you want. For example, the first attempt might produce something like this:




1. If the curve is not already selected, click **Select/Move/Resize**  and then click the curve.
2. On the Editing toolbar, click **Edit Nodes** . This will show all the nodes of the polyline that can be modified:





3. Click the third node, and you will see the node selected and the control lines appear:



4. Drag the control lines, then select and modify the other nodes until the curve looks as you like.

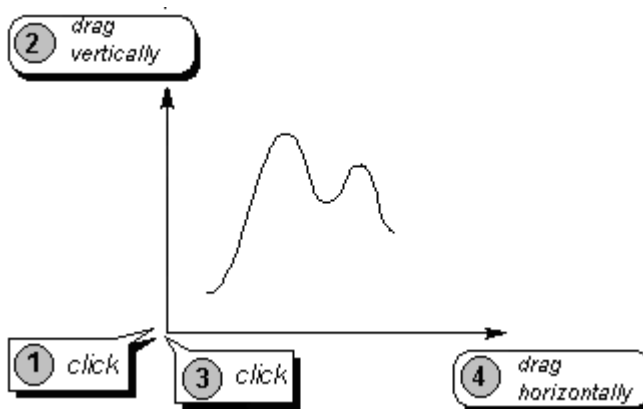
**Tip** When using the **Edit Nodes**  tool, you can manipulate nodes using the buttons on the **Node** toolbar that appears. For example, you can select several nodes by clicking on them when holding down SHIFT, and then align them by choosing the corresponding button on the toolbar.



## 9.2.3 Drawing the X and Y axes




To accomplish drawing of a reaction diagram, the axes are required. Make sure that the **Line**  and **Arrow**  tools are active.

1. From the **Tools** menu, choose **Arrow Style Panel**. On the **Arrow** panel that appears, from the **Arrow Type** drop-down list , choose the one-way arrow .
2. From the **Options** menu, choose **Snap on Grid** and/or **Show Grid** to make your drawing easier.
3. Click at the origin of coordinates and drag the mouse up vertically to draw the Y-axis.


4. Click at the origin of coordinates and drag the mouse horizontally to the right to draw the X-axis.



5. Add inscriptions *Energy* and *Reaction Coordinate* using the **Text**  and **Rotate 90°**  tools.

! Here's a challenge. Use the **Text**  tool to print a word in the workspace. Select it and change its font size to, say, 36 points, and its color to yellow. Now use the **Polyline**  tool to write the word over top. (Hint: "write" the word as best as you can and then use the **Edit Nodes**  tool liberally.)

Chemistry

6. On the General toolbar, click **New Page** .

### 9.3 Drawing Different Kinds of Orbitals




This section is based on the movie **orbital.exe** which can be downloaded from our Web site or found in the Movies folder.

#### 9.3.1 Drawing a p-orbital

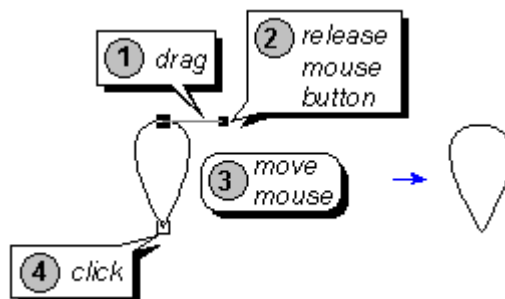
We are going to draw the following orbital:





Make sure you are in the Draw mode and, on the Drawing toolbar, click **Polygon** .

1. Drag horizontally to the right from the starting point of the orbital to stretch the control line.

2. Release the mouse button.
3. Move the mouse down to draw the body of the orbital.
4. Click to fix the orbital.

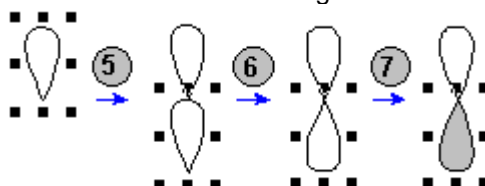



**Note** If the shape of the curve is not what you want, use the **Edit Nodes**  tool.



5. Right-click twice to finish drawing the orbital and to quickly switch to the **Select/Move/Resize**  tool. Point to the selected orbital; and drag it down holding down CTRL to make a copy of the drawn orbital.
6. On the Editing toolbar, click **Flip Top to Bottom**  to flip the lower segment of the orbital. Align the segments by moving them.

**Tip** To align the elements more precisely, make sure that the **Snap on Grid** is not selected on the **Options** menu.

7. Click the gray color on the Color Palette to change the fill color of the orbital segment.

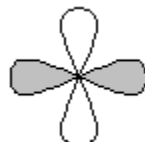


**Tip** To quickly center the orbital segments, select them and click **Center Horizontally** .

8. Select both segments of the orbital and, on the Editing toolbar, click **Group** . Now you can manipulate the segments as a single object, e.g., rotate using the **Select/Move/Rotate**  tool.


### 9.3.2 Drawing a d-orbital

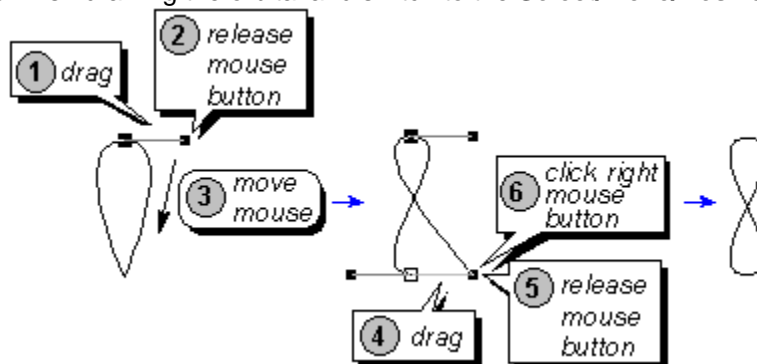
In this section, we will draw the orbital:




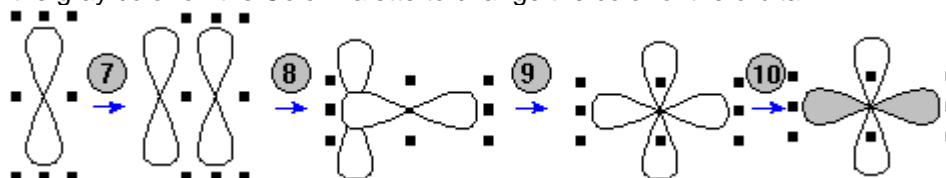
Make sure you are in the Draw mode and select the **Polygon**  tool.


**Tip** From the **Options** menu, choose **Snap on Grid** before drawing to ease the drawing of the symmetrical orbital.

1. Drag horizontally to the right from the starting point of the orbital to stretch the control line.
2. Release the mouse button.
3. Move the mouse down to draw the body of the orbital.
4. Drag horizontally to the right to stretch the control lines. Note that to make the two segments of the orbital identical, make the lengths of the control lines equal.
5. Release the mouse button.
6. Right-click to finish drawing the orbital and switch to the **Select/Move/Resize**  tool.



7. Select the orbital and, holding down CTRL, drag to make a copy of it.
8. Click **Rotate 90°**  to rotate the copy of the orbital.
9. Drag the copy as shown below.
10. Click the gray color on the Color Palette to change the color of the orbital:





**Tip** To quickly center the orbitals, select them and click the **Center Horizontally**  button.

11. Select both orbitals and click **Group** . Now you can manipulate the orbitals as a single object, e.g., rotate using the **Select/Move/Rotate**  tool.

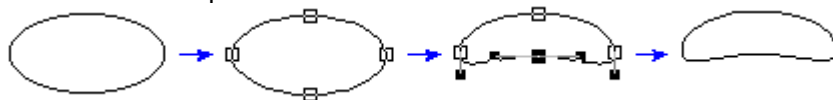
### 9.3.3 Drawing a pi-type orbital



We will draw the following orbital:




1. On the Drawing toolbar, click **Ellipse**  and drag in the workspace to draw an ellipse.
2. From the **Object** menu, choose **Convert to Polyline**.
3. On the Editing toolbar, click **Edit Nodes** .



4. Drag the lowest node up.



5. Right-click to switch to the **Select/Move/Resize**  tool, then select the orbital by clicking its contour, and then, holding down CTRL, drag to make a copy of it.
6. Click **Flip Top to Bottom**  to flip the lower orbital.
7. Point to the gray color button in the **Color Palette** and click on the left mouse button to change the color of the orbital.



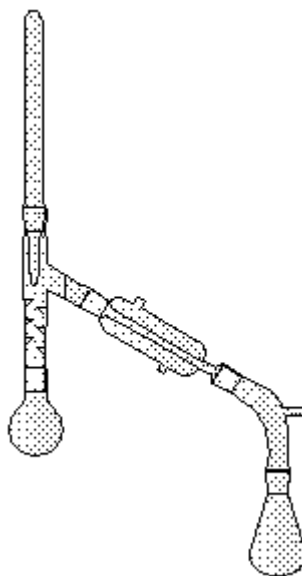
**Tip** To quickly center the orbitals, select them and click **Center Horizontally** .



8. Select both orbitals and, on the Editing toolbar, click **Group** . Now you can manipulate them as a single object.
9. On the General toolbar, click **New Page** .



## 9.4 Drawing Vacuum Distillation Apparatus

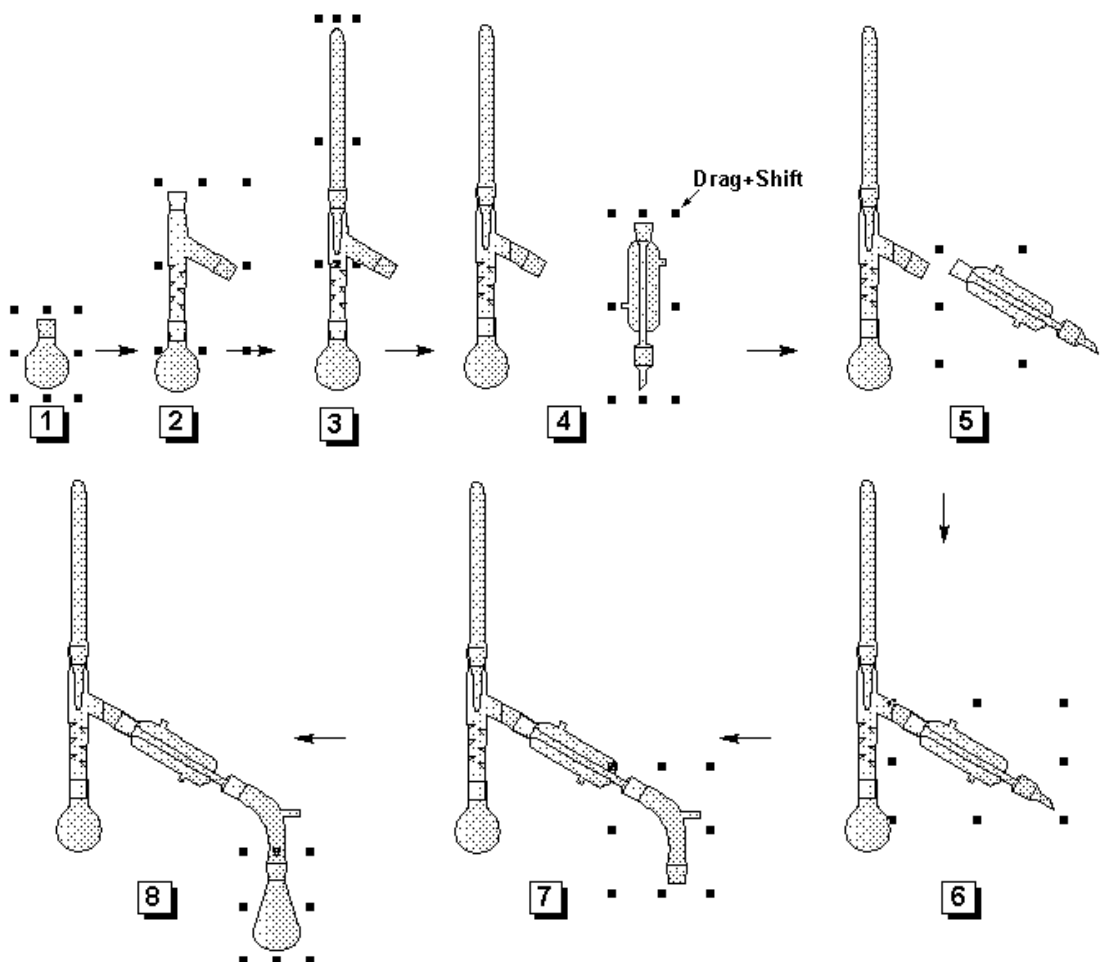


This section is based on the movie **apparatus.exe** which can be downloaded from our Web site or found in the \\MOVIES folder.



1. Switch to the **Draw** mode and set 50% zoom, then click **New Page**  to open a new empty page.
2. In the **Template Window** , from the list of templates, choose **Lab Kit**.

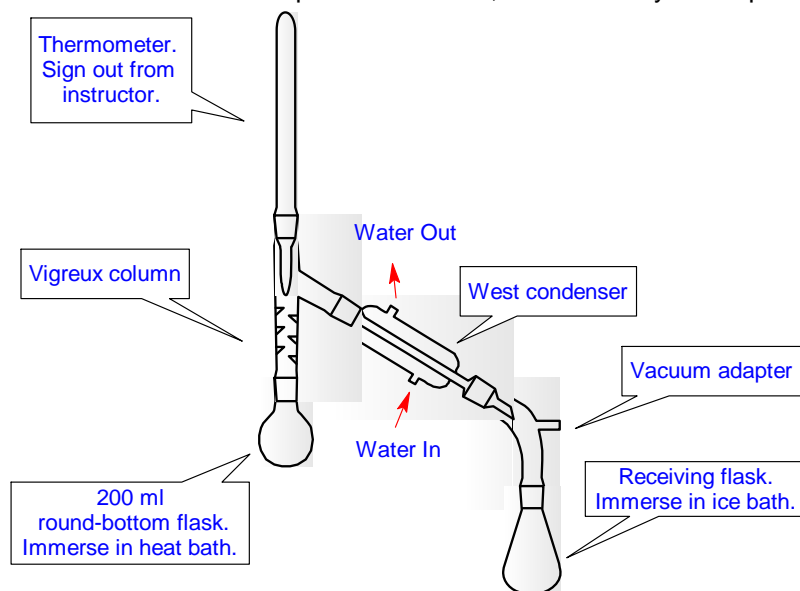
3. Select the round-bottom flask by clicking (view the scheme below). Click in the workspace to add the selected template, and then right-click to hide the template shadow.
4. Open the Template window. Select the three-way adapter (Vigreux distillation column with connecting adapter). Connect it to the flask by clicking and right-click to hide the template shadow.
5. From the Template window, choose the thermometer, and connect it by clicking as shown. Hide the template shadow.
6. From the Template window, choose the Liebig condenser and place it on the workspace near the apparatus by clicking. Right-click to hide the template shadow and switch to the **Select/Move/Resize**  tool.
7. Click any selection handle (black squares surrounding the distillation column) to quickly switch to the **Select/Move/Rotate**  tool. Rotate the selected object about  $73^{\circ}$  counter-clockwise by dragging any selection handle. The informative cursor will show you the angle of rotation (if the corresponding option has been selected in the **Preferences** dialog box (**General** tab)).
8. Drag the column and attach it to the apparatus.
9. From the Template window, choose the vacuum-distilling adapter and attach it to the apparatus.
10. Complete the drawing by connecting the receiving flask (round-bottom flask).



### 9.4.1 Annotating a Diagram

ACD/ChemSketch enables you to draw many elegant and detailed set-ups of your glassware apparatus. The Lab Kit template includes burettes, beakers, hot plates, bunsen burners, etc. so that you will be able to draw an experiment from start to finish.

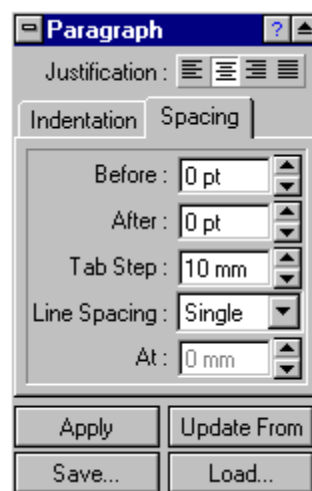
Let's say that you are preparing the diagram for an instruction manual in an undergraduate laboratory. You might want to direct the attention of the students to certain aspects of the set up, possibly even to remind them what the parts are named, or where they are kept in the lab:




#### 9.4.1.1 Adding Text Captions

From this section, you'll find out how to add callouts to the vacuum distillation apparatus:


1. Firstly, let us set the font to be used for the text. From the **Tools** menu, choose **Font Panel** and **Paragraph Panel**. Specify the following settings and close the panels:



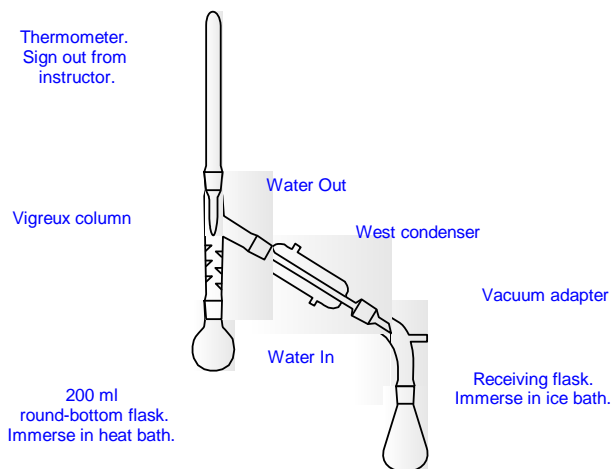
- On the Drawing toolbar, click **Text**  and click to the left of the thermometer. In the text box that appears type *Thermometer. Sign out from instructor.* To narrow the text box, drag its right border:



- Click outside of the text box to leave the Text mode and to fix the caption.


**Tip** To edit the text later, on the Editing toolbar, click **Text**  again, and click the text to be edited.

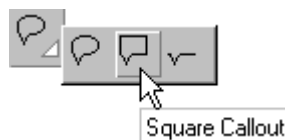
- Repeat steps 2 and 3 to add other captions.
- If necessary move the captions to arrange them around the apparatus:



#### 9.4.1.2 Inserting Callouts

Now we are going to include the captions into callouts.

- On the left Drawing toolbar, click the right-bottom corner (i.e., the small white triangle) of **Callout**  to expand it into more buttons. From the available styles, choose the square callout type:






- As you point to different objects on the workspace, you will see the callout shadow appearing around them. Point to the text caption so the that callout shadow appears around it and click to fix it:



- Subsequently point to other captions and click to fix the callouts. To leave the callout mode, right-click in the workspace.

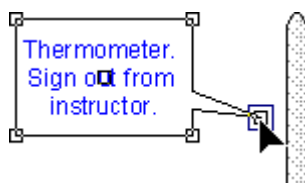
### 9.4.1.3 Reshaping Callouts

Now we are going to modify the callouts so that their pointing ends are directed at the required objects.


- Select any of the drawn callouts by clicking and then clicking **Edit Nodes**  on the upper Editing toolbar. The nodes appear on the callout:




- Drag the lowest node to a new location so that it correctly points to the object you want to annotate:



**Tip** Dragging the corner nodes modifies the size of the callout.

- Without leaving the Edit Nodes mode, click another callout and repeat step 2 as needed.
- As soon as all the callouts are redirected as necessary, right-click in the workspace to leave the Edit Nodes mode.
- Using the **Draw Arrow**  tool, add arrows to indicate the water inlets and outlets.
- Select both arrows and double-click to display the Objects Panel. Set the pen color to red and click **Apply**.

### 9.4.1.4 Grouping/Ungrouping Elements

To be able to manipulate this picture as a single object, select all its components by pressing CTRL+A and click **Group**  on the Editing toolbar. Now you can move and/or resize the picture as a whole without the risk of losing or leaving behind any of its elements.

If later you decide to edit any of the picture components, select the picture and release **Group**






## 9.5 Drawing a Two-chain DNA Strand

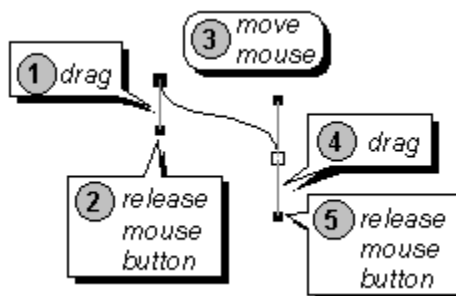


This section is based on the movie **dna\_ch.exe** which can be downloaded from our Web site or found in the \\MOVIES folder.



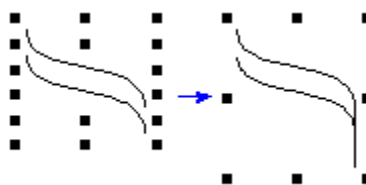
Make sure you are in the Draw mode.

1. On the General toolbar, click **New Page** .
2. On the Drawing toolbar, click **Polyline** .
3. Drag vertically down from the starting point of the curve to stretch the control line.
4. Release the mouse button.
5. Move the mouse to the right to draw the curve.
6. Drag vertically down to stretch the control lines. By changing the length of the control lines you can modify the form of the curve.
7. Release the mouse button and right-click twice to finish drawing the curve and to activate the **Select/Move/Resize**  tool.






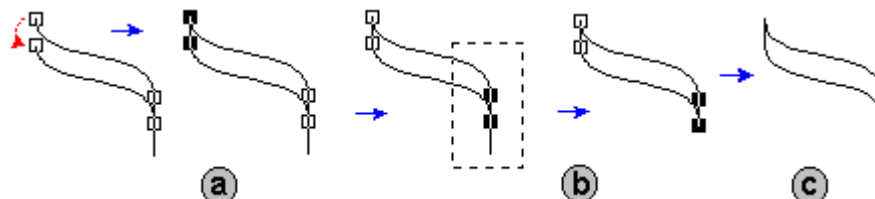
8. Point to the selected curve and, while holding down CTRL+SHIFT, drag it down (holding down CTRL while dragging leaves behind an instant copy of the object and holding down SHIFT forces the object to move strictly vertically or horizontally).
9. Select both curves by dragging the selection rectangle around them or by clicking each of the curves while holding down SHIFT, then from the **Object** menu, choose **Connect Lines** to

connect the right ends of the curves.



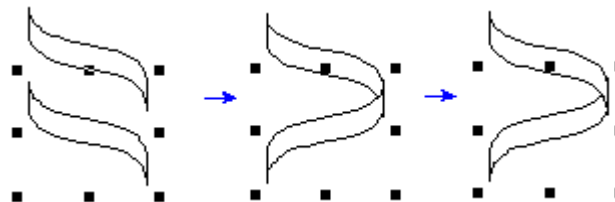
10. On the Editing toolbar, click **Edit Nodes** . Proceed with the following to draw a segment:

- Click **Connect Vertices**  to connect the end nodes with a line.
- Select the right two nodes by dragging the selection rectangle around them and, on the Edit Nodes toolbar, click **Convert to Line** .
- Right-click to leave the **Edit Nodes** mode and to switch to the **Select/Move/Resize** tool .




11. Make a copy of the obtained segment by dragging it with CTRL+SHIFT as described in step 6.

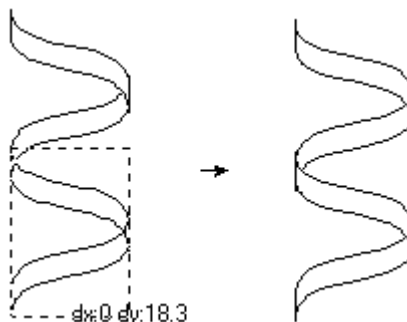
On the Editing toolbar, click **Flip Left to Right**  to flip the segment and then click **Send to Back**  to send the segment to the background.



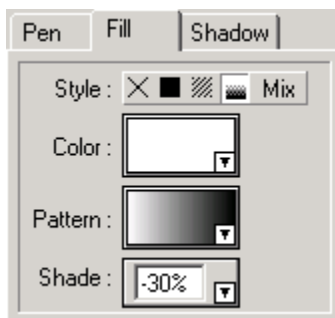
**Tip** It may take some time to correctly position the segments by manually moving them. To align their position automatically, select both segments and apply the **Center**

**Horizontally** tool  to the segments.

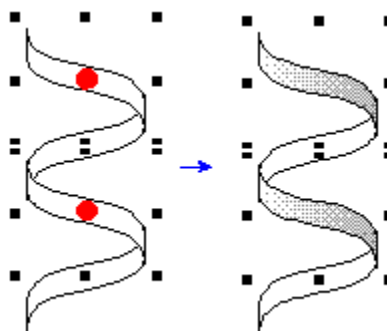
12. Select both segments by dragging or clicking while holding down SHIFT and make a copy (hold down CTRL while dragging). Correct the position using the directions in the previous step:



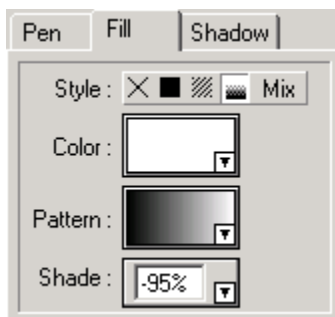
13. Select the segments marked with bullets in the picture below by clicking them while holding down SHIFT. Double-click any of them to open the **Objects** panel. On the **Fill** tab, specify the following settings:



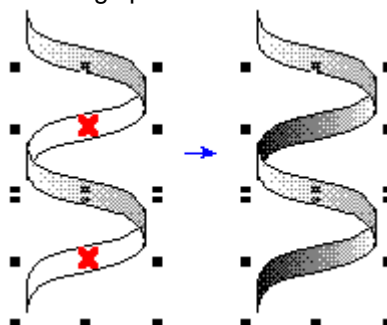
and click **Apply**:





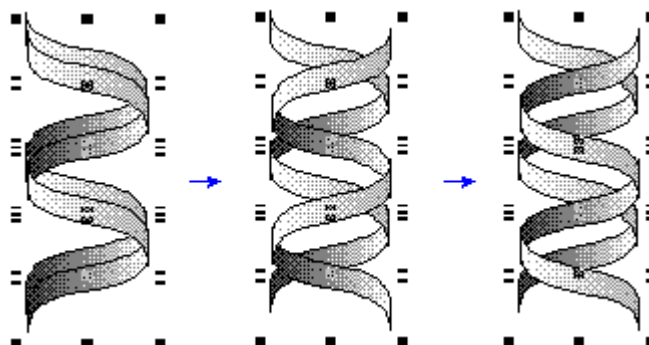
14. Select the other two segments (they are marked with crosses in the figure below) and specify the following settings on the **Objects** panel:




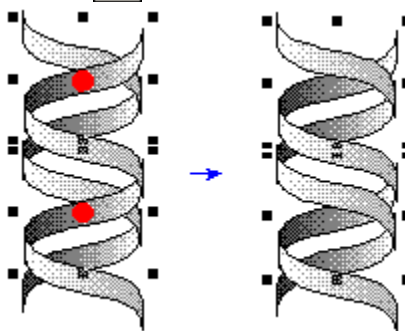
and click **Apply** to obtain the following spiral:



15. Select the whole spiral by dragging the selection rectangle so that it includes all the spiral segments and make a copy of it by dragging while holding down CTRL. Click **Flip Left to Right**  and then **Flip Top to Bottom** .



16. Select the segments marked with bullets in the picture below by clicking while holding down SHIFT, and then click **Send to Back** .



17. Select all the segments and group them.

## 9.6 Drawing Lipids and Micelles




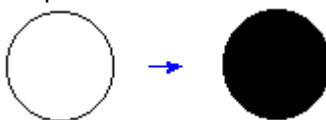
This section is based on the movie **lipid.exe** which can be downloaded from our Web site or found in the Movies folder.


### 9.6.1 Drawing the lipid

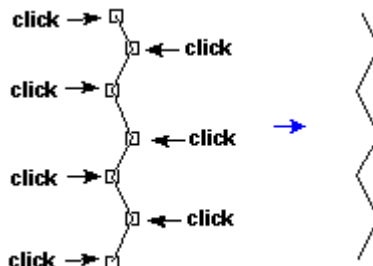


Make sure you are in the Draw mode.





1. On the Drawing toolbar, click **Ellipse** . Drag in the workspace while holding down SHIFT to draw a circle.
2. Click the black color of the Color palette to fill the circle.

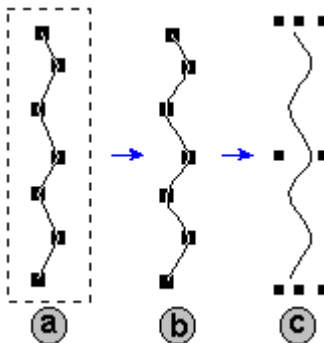


3. Click **Polyline** . Click repeatedly in the workspace near the circle to draw the carbonic tail and right-click to finish drawing.



**Tip** To easily draw the symmetric zigzag line, you may previously select the **Snap on Grid** and/or **Show Grid** from the **Options** menu.


4. Click **Edit Nodes**  and smooth the zigzag line in the following way:
  - a. Select all the nodes of the drawn polyline by dragging the selection rectangle around it. Note that selected nodes become black.
  - b. Click **Convert to Curve**  and then **Smooth** .
  - c. Right-click to switch to the **Select/Move/Resize**  tool.






5. Point to the curve and drag it holding down CTRL to leave the copy of the curve behind.

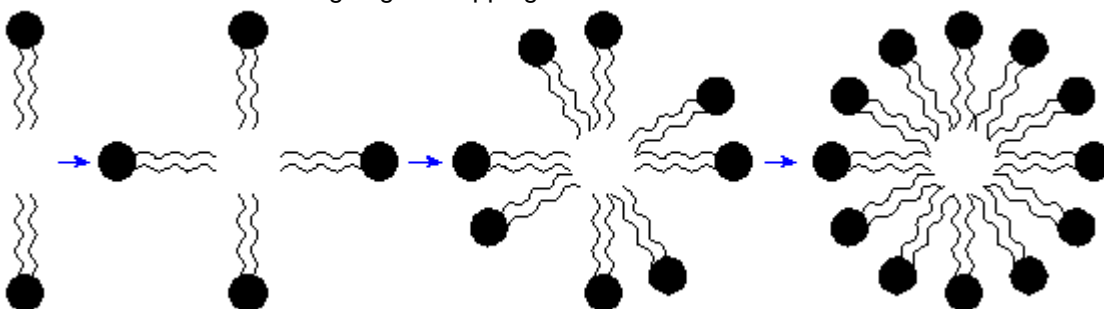
6. Arrange the tails as shown by dragging them.



**Tip** If you select all the elements of the phospholipid and click **Group** , you will be able to manipulate them as a single object, e.g., rotate it using the

**Select/Move/Rotate**  tool.

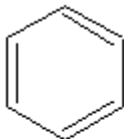
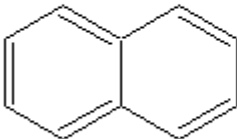
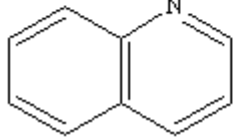
! Try drawing the micelle picture using the copying feature (holding down CTRL while dragging), **Group** , **Rotate 90°** , and **Select/Move/Rotate**  as well as the aligning and flipping tools:



## 9.7 Creating Tables


Starting from version 7.0, ACD/ChemSketch offers an enhanced tool for drawing and managing tables. In this section, you will learn how to insert the table, add data to the table, and edit table.

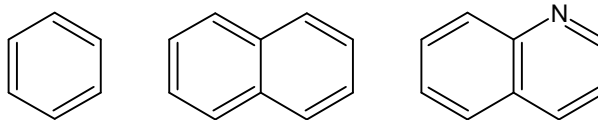
As an example we will draw the following table:

Structure	Name	Properties
	Benzene	Composition = C(92.26%) H(7.74%) Density = $0.873 \pm 0.06 \text{ g/cm}^3$
	Naphthalene	Composition = C(93.71%) H(6.29%) Density = $1.037 \pm 0.06 \text{ g/cm}^3$
	Quinoline	Composition = C(83.69%) H(5.46%) N(10.84%) Density = $1.106 \pm 0.06 \text{ g/cm}^3$

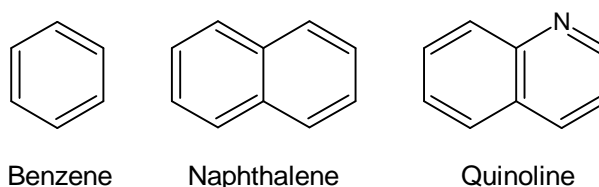
### 9.7.1 Drawing the Table Contents

First of all, we should draw the contents for our table:

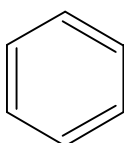
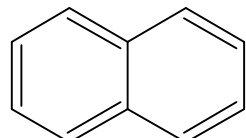
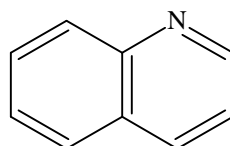
1. Switch to the Structure mode.
2. Draw the structures of benzene, naphthalene, and quinoline using the technique described in the previous sections or find these structures in the **Dictionary** :




3. Switch to the Draw mode and, using the **Artistic Text** tool , insert the names for each of the structures:



4. Now calculate all or some of the properties for each of them (for more details on how to calculate properties, refer to Chapter 6). If necessary, move the structures and text for better viewing. You should obtain something like the following:

	Benzene	Composition = C(92.26%) H(7.74%) Density = $0.873 \pm 0.06 \text{ g/cm}^3$
	Naphthalene	Composition = C(93.71%) H(6.29%) Density = $1.037 \pm 0.06 \text{ g/cm}^3$
	Quinoline	Composition = C(83.69%) H(5.46%) N(10.84%) Density = $1.106 \pm 0.06 \text{ g/cm}^3$


5. Choose the **Artistic Text**  tool. Click the empty space and type '*Structure*'. Then click outside the text box. In the similar way insert '*Name*' and '*Properties*'. These are going to be the table headings:

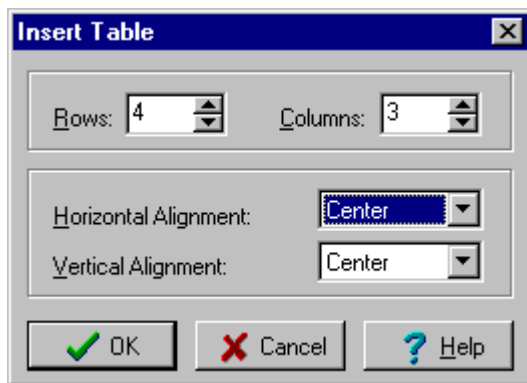
Structure      Name      Properties



### 9.7.2 Inserting Table

Now we can add the borders to the table contents:


1. On the left toolbar, click **Table**  and drag in the empty workspace until you define the approximate size for your table. The **Insert Table** dialog box appears. Set the number of rows and columns to 4 and 3:



2. Click **OK**. The empty table is inserted. Right-click to leave the table drawing mode.

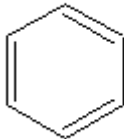
### 9.7.3 Placing Data into Table


After the table is drawn, we can fill it in with the previously specified data:

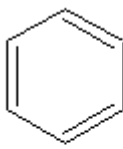
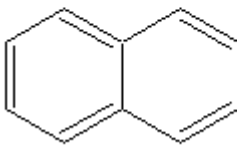
1. Make sure that the **Select/Move/Resize**  tool is enabled and drag the 'Structure' notice to the upper leftmost cell of the table so that it is placed somewhere in the center of the cell. As you release the mouse button the text is automatically added to the cell and the cell is resized to fit the text (this is the first way to add the data to the table):

Structure		

2. Now drag the benzene structure to the cell right below the Structure heading. Note that the cell size changes correspondingly:

Structure	
	

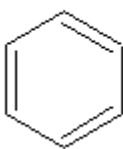
3. Another way of filling in is as follows. Click the naphthalene structure to select it, hold down SHIFT and click an empty cell below the cell with the benzene to select both objects. On the Editing toolbar, click **Group** . The structure is automatically placed into the cell and the cell is fitted to the structure size:

Structure	
	
	

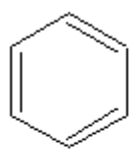
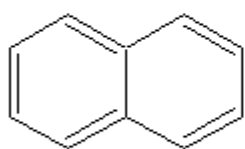
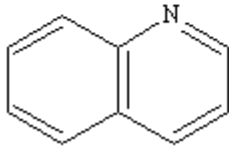
4. You can also add several objects to table at once. Click the Benzene text, then hold down SHIFT and click the properties related to benzene to select both objects.


■ ■ ■ ■ ■  
 ■ Benzene ■ Composition = C(92.26%) H(7.74%) ■  
 ■ ■ ■ Density = 0.873 ± 0.06 g/cm<sup>3</sup> ■  
 ■ ■ ■ ■ ■

5. Drag them to place so that they are located over the two cells to the right of the benzene structure and release the mouse button. The two objects are placed into separate cells:

Structure		
	Benzene	Composition = C(92.26%) H(7.74%) Density = 0.873 ± 0.06 g/cm <sup>3</sup>


6. Add other objects to the cells either by dragging or selecting and grouping. You should obtain something like the following:

Structure	Name	Properties
	Benzene	Composition = C(92.26%) H(7.74%) Density = 0.873 ± 0.06 g/cm <sup>3</sup>
	Naphthalene	Composition = C(93.71%) H(6.29%) Density = 1.037 ± 0.06 g/cm <sup>3</sup>
	Quinoline	Composition = C(83.69%) H(5.46%) N(10.84%) Density = 1.106 ± 0.06 g/cm <sup>3</sup>


**Tip** If the text or any of the objects are not fully visible, enlarge the table box (the dashed line around the table cells). Select the table box and drag the corner selection handle  to resize the table.

### 9.7.4 Modifying Table Contents

Now we are going to modify the formatting of the table contents.

1. Make sure that the **Select/Move/Resize**  tool is active and drag over the upper row of cells to select them:

Structure	Name	Properties
-----------	------	------------

2. On the Editing toolbar, click **Group**  to release it. This will ungroup each of the cells and their contents. You can see that now only the text is selected:


Structure	Name	Properties
-----------	------	------------

3. Double-click any of the text portions to display the **Objects Panel**. On the **Font** tab, select the **Bold** check box, set the size to 12, and click **Apply**.

<b>Structure</b>	<b>Name</b>	<b>Properties</b>
------------------	-------------	-------------------

4. Close the **Objects Panel**.
5. Click somewhere in the empty space to remove selection.
6. To place the text back into the table cell, select the text, for example, start with the 'Structure' notice, hold down SHIFT and select the cell where the selected text should be placed:

Structure
-----------


7. Click **Group** . The cell and contents are now grouped:

Structure
-----------

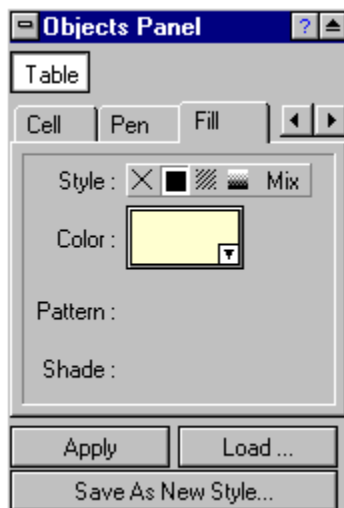
8. Another way of grouping is to point to the text and drag it a little so that it is placed somewhere in the center of the cell, as you release the button, the text will be automatically grouped with the cell. To understand whether the object and the corresponding cell are grouped, point to the object, if the whole cell is surrounded with the selection frame, but not the object only, the object has been inserted into the cell. Using any of the methods described, place other headings into the cells.

### 9.7.5 Editing Table View


Finally, we can modify the table view:

1. Make sure that the **Select/Move/Resize**  tool is selected and drag over the upper row to select it.

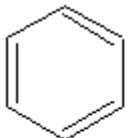
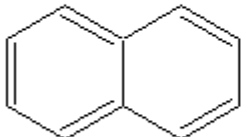
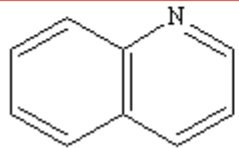
2. Double-click the selection to display the **Objects Panel**. If the **Fill** tab is not visible, click the right arrow to display it and switch to the tab. Set the color to, for example, ivory:



3. Click **Apply**: The selected cells are filled with ivory color:

Structure	Name	Properties
		

4. Close the **Objects Panel**.
5. Select the entire table and double-click it to display the **Objects Panel** (note that, on the **Fill** tab, the color is set to mixed). Switch to the **Pen** tab and change the color to crimson. Click **Apply**.

Structure	Name	Properties
	Benzene	Composition = C(92.26%) H(7.74%) Density = $0.873 \pm 0.06 \text{ g/cm}^3$
	Naphthalene	Composition = C(93.71%) H(6.29%) Density = $1.037 \pm 0.06 \text{ g/cm}^3$
	Quinoline	Composition = C(83.69%) H(5.46%) N(10.84%) Density = $1.106 \pm 0.06 \text{ g/cm}^3$

6. Close the **Objects Panel** and save the file.

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## 10. Managing Documents

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If you have worked over the material described in the previous chapters, you should have several pages with various drawings. In this chapter, we are going to practise some manipulations that concern the whole document.

In this chapter, you will learn how to:

- Insert headers and footers
- Convert the document to Adobe PDF format—**Commercial version only!**
- Create a poster

The sections below do not pertain to some particular example and can be applied to any of your ACD/ChemSketch documents.






### 10.1 Inserting Headers and Footers

Starting from version 8.0, you can insert headers and footers for all the pages in your document. You only have to define the text or picture to be inserted in one page and the rest of the pages will be provided with the same pattern.


1. On the **Pages** menu, point to **Headers and Footers**, and then choose **Edit**. The corresponding toolbar appears



and at the top of the page the text editing box appears.

2. Type the text to be a header of the page, for example, "ACD/ChemSketch".
3. On the Headers and Footers toolbar, click **Go to Next Text** , one more text box appears at the center of the page's header. Type "Author:".
4. Now click **Insert AutoText**  on the toolbar and choose **Author**. Your login name is automatically inserted.
5. Click **Go to Next Text**  again to insert one more text box to the right of the page's header. Click **Insert AutoText**  and choose **Page X of Y**, the corresponding auto text is inserted. If you want to add more data to the page footer, click **Go to Next Text** .

**Note** You can also insert any drawings to be present either in the header or footer. When in the Header and Footer Editing mode, draw or insert the picture using the ChemSketch tools and place it to the required position. As you leave this mode, the corresponding picture will be available in all the pages of your document.

6. As soon as the required data is inserted, leave the Header and Footer Editing mode by closing the toolbar. Click **Close** .
7. Switch between the pages to view the headers inserted.


## 10.2 Converting to Adobe PDF

ACD/ChemSketch now includes a tool for converting ACD/ChemSketch files (.SK2) to the Adobe PDF format. As soon as you have drawn some graphical objects as described in the previous chapters, you can try to convert your document to the Adobe PDF format. Note that this feature is only available in the commercial version of ACD/ChemSketch.

**Note** To be able to export to PDF from ACD/ChemSketch, you do not have to install Adobe Acrobat or Acrobat Reader on your computer, but to view PDF files you should have any of them. You can find the free version of the Adobe Acrobat Reader in the ACD/Labs installation folder.

1. Make sure that the objects and structures are arranged on the screen in the way you want to see them in the PDF file.

**Tip** Click **Full Page**  to view the whole page.

2. Click **Export to PDF** . The program will prompt you for the location and name of your .PDF file.
3. Type the name, e.g. *Chapter10.pdf*, and click **OK**.
4. As soon as the conversion is finished, find the newly created file and open it with Adobe Acrobat Reader to view the results.

**Note** Some objects inserted via the OLE server (from the **Edit** menu, choose **Insert Object**) may not be converted into PDF. In this case, a message box appears informing you of this.

## 10.3 Creating a Poster

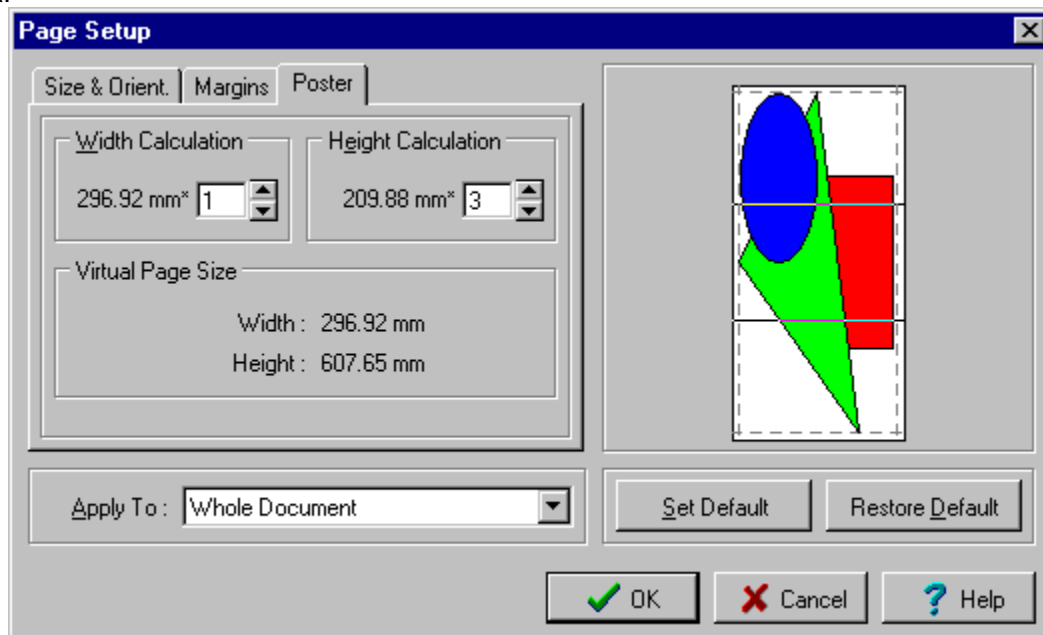
Using ACD/ChemSketch you can quickly draw a poster and print it on paper of any format. ACD/ChemSketch will automatically separate the poster into pages; the only thing you have to do (besides design) is to attach them.




This section is based on the movie **poster.exe** which can be downloaded from our Web site or found in the \\MOVIES folder.


1. From the **File** menu, choose **Page Setup**.
2. On the **Size & Orient.** tab, set the paper format and choose the **Landscape** option.

3. Select the **Poster** tab. Set the number of standard pages you want your poster to consist of. Note that you can see the automatically calculated size of the poster in the **Virtual Page Size** area:



4. On the **Margins** tab, set the page margins and click **OK**.
5. Draw your poster using the tools in the Structure and Draw modes. Click **Full Page**  to see the general layout as you prepare it.

**Note** You can use **Paste** and **Paste Special** from the **Edit** menu to insert objects (text, pictures, etc.) created in other Windows applications. You can also edit these objects using OLE.

6. If you want to see how your poster will be divided into individual pages while being printed, from the **Options** menu, choose **Preferences** and in the **Preferences** dialog box, **General** tab, **Borders** area, select the **Printable Area** check box.
7. From the **File** menu, choose **Print** or click **Print**  on the General toolbar to print your poster and attach the pages.

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## 11. Working with Styles in Structure Mode

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### 11.1 Objectives

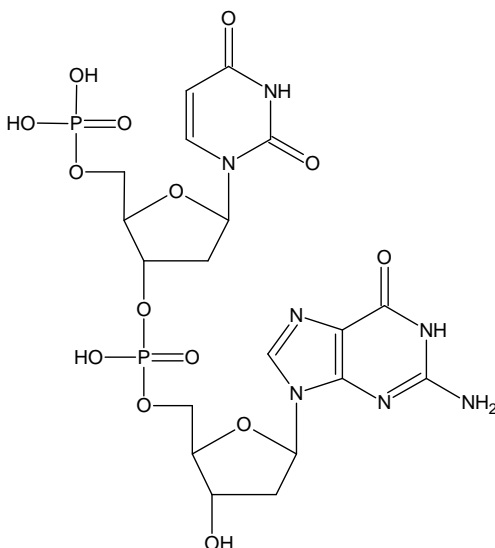
If you often display your structure with a particular set of attributes, such as size of font, style of font, thickness of bond line, etc. You can make ACD/ChemSketch remember these settings by saving them altogether as a *Style*. This is especially helpful if you want to display structures one way when working with them, but make them conform to a particular journal style when submitting a paper for publication.

In this chapter, you will learn how to:

- Change the style of structures
- Save your style
- Apply an existing style
- Set a default style

### 11.2 Changing Style of Structures

A style is a collection of attributes for display (atom and bond for structures; pen, arrow, fill, font, paragraph for objects and text) to which you can assign a name and save.




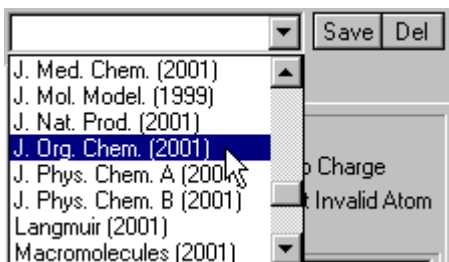
**Tip** This structure can be drawn with the help of the **Template window (DNA/RNA Kit tab)**. Use the 2-deoxyribose-5-phosphate, uracil, and guanine components. When attaching a template, hold down SHIFT when clicking to attach it without creating an additional bond. For more details on how to use the Template window, refer to Section 5.5



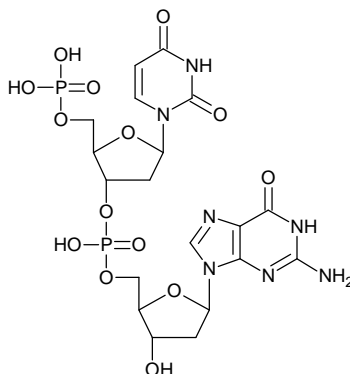
### 11.2.1 Applying a Journal Style

Let's say that you have written a scientific article and, to accompany it, you want to submit this drawing of the structure to the *Journal of Organic Chemistry*.

1. Select the structure using the **Select/Move**  tool.
2. Point to one of the selection markers so that they turn from small outlined squares to solid black squares. Double-click and the **Properties** dialog box appears.
3. In the **Style** box, select **J. Org Chem (2002)**:



4. Click **Apply** and you will see the display of the structure changes to reflect that journal's style. Click beside the structure to unselect it, so you can see it more clearly:



5. From the **File** menu, choose **Save As** and write your structure to a file as DNAFRAG2.SK2.
6. Select the whole structure again, and in the **Properties** dialog box, from the **Style** list, select **Normal**.
7. Click **Apply** and the structure should appear as before.

### 11.2.2 Preparing for Publication

In addition to making your structural drawing conform to the guidelines of a particular journal, there are many other matters to arrange during manuscript preparation. For this reason, Advanced Chemistry Development has included **Instructions for Authors**, a hyperlinked list of guidelines for over 80 journals.



1. For example, from the **Help** menu, choose **Instructions for Authors**.
2. Find the **Journal of Organic Chemistry** in the list.
3. Click the link to the Adobe PDF file to display the corresponding file.

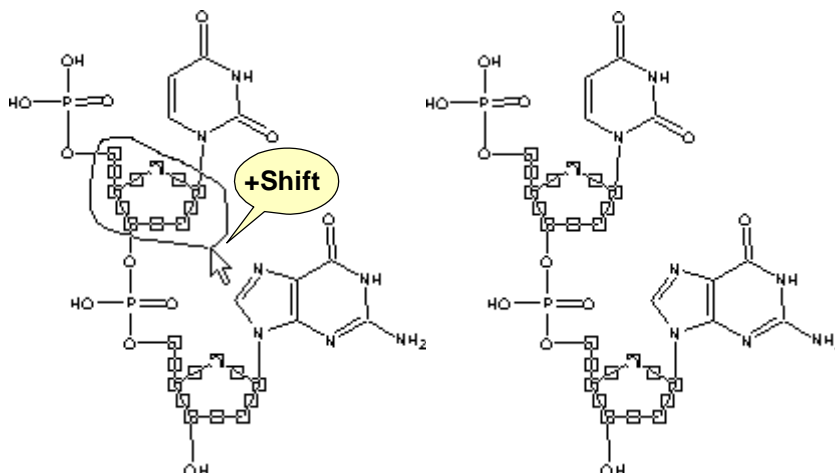
4. Click **Contents** to return to the list of other journals so you can view their guidelines too.

**Note** Not all journals have explicit instructions for structural drawings, and so they do not appear as a definite style listed in the **Structure Properties** dialog box.

## 11.3 Creating Your Own Style

Let's say that you want to make a presentation in which you want to colorfully distinguish between the sugar, phosphate, and amino acid groups of the portion of DNA you are describing.

1. Open the file DNAFRAG.SK2 (or draw the DNA fragment shown above in Section 5.5.1) and make sure that you are in the Structure mode.
2. Switch to the **Lasso On** tool  and click **Select/Move** .
3. Select the sugar components by dragging around them (hold down SHIFT when selecting separate components):

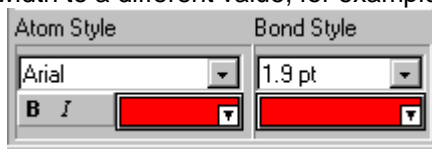


4. Point to any part of the selected fragment so that the selection squares become black. Double-click to display the **Properties** panel.

### 11.3.1 User-defined Style: Sugar

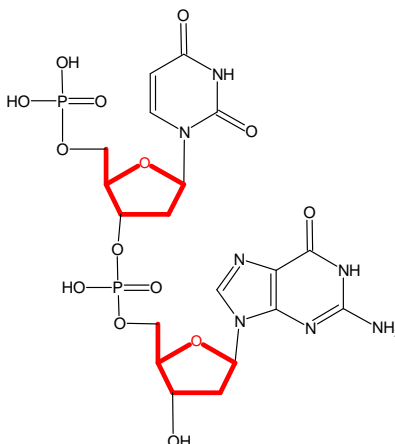
Now we will define our own style for the sugar components:

1. In the **Atom Style** and **Bond Style** areas, specify the color for the selected fragments, for example, red. Set the bond width to a different value, for example, 1.9 pt.



**Note** Units of measurement used in most of the panels within ACD/ChemSketch correspond to those set in the **Preferences** dialog box (**Options** menu). You may set values for width, length, etc. in points/inches/millimeters/centimeters. Type the values and add the unit you want (pt/in/mm/cm), e.g., 5 pt. The values will be recalculated in the corresponding units of measurement.

2. Click **Apply**. As you can see, the selected segments are colored with red now:



3. To save this style for future use, in the Style box of the **Properties** dialog box, type *Sugar* and click **Save**:

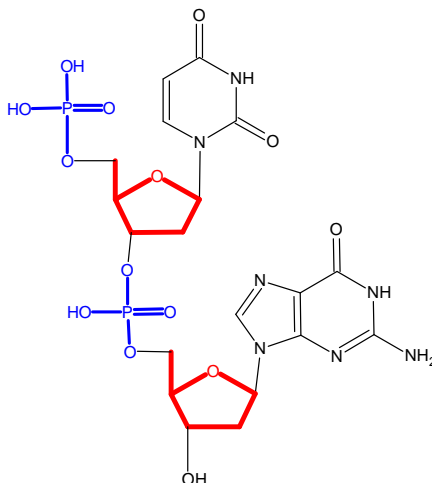


4. You will be prompted whether you want to save this user-defined style. Click **Yes**.

### 11.3.2 User-defined Style: Phosphate

In this section, we will define our own style for the phosphate components:

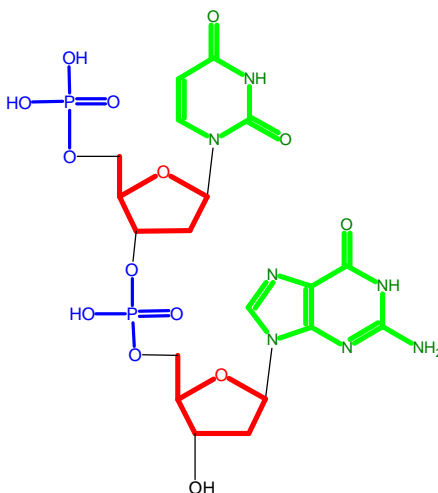
1. Similarly, select the phosphate part of the structure, and define a thick bond width and blue color for the bonds and atom fonts.
2. Save this style as *Phosphate* and then click **Apply** to apply it to the structure:



### 11.3.3 User-defined Style: Base

We can also define our own style for the bases:

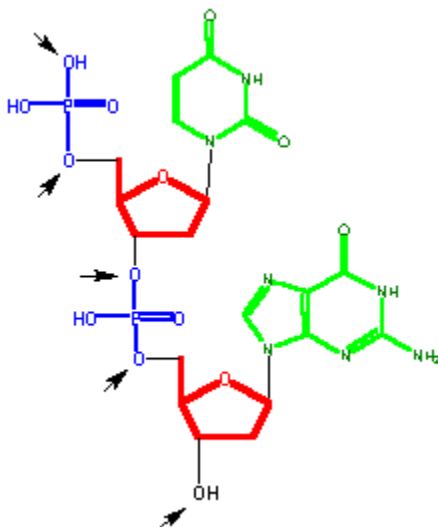
1. For the bases, set the color of the atom symbols to dark green and the bonds to neon green.
2. Save this style as *Base* and then click **Apply** to apply it to the structure:



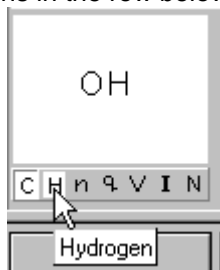
### 11.3.4 User-defined Style: Highlight

Perhaps, during the course of your presentation you want to draw the attention of the audience to the oxygen atoms. We will create a fourth style, *Highlight*, for this.

1. Use SHIFT+ click to select the oxygen atoms indicated below with the arrows:



2. Double-click any of the selected atoms, and, on the **Properties** panel, switch to the **Atom** tab.
3. To change the color and size of both the atom symbol (oxygen in this case) and hydrogen, click the corresponding buttons in the row below the preview area holding down SHIFT.



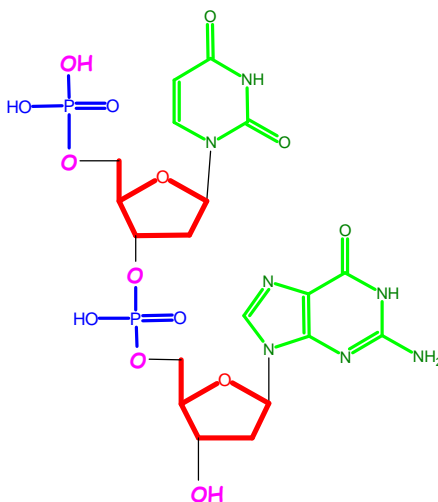
**Note** You may also change other atom attributes (hydrogen index, charge, valence, isotope, numbering) by clicking the corresponding buttons.

4. Change the color, atom size, and other attributes, for example, to the following settings:



**Note** In a similar manner, you may change the bond attributes.


5. Click **Apply** to obtain the following structure:

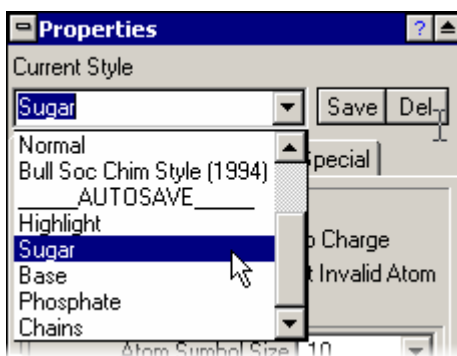


6. Save the style as *Highlight*.

## 11.4 Applying Existing Styles

To practice applying the styles you have just created, open DNAFRAG2.SK2.

1. Use the **Lasso** tool  to select the five-membered sugars as shown in Section 11.3.
2. Double-click those substructure fragments or from the **Tools** menu, choose **Structure Properties**.
3. On the **Properties** panel that appears, from the Styles box, choose **Sugar**:



4. Click **Apply**. The chosen style will be applied to the selected structure or fragment.
5. Choose the phosphate groups. From the **Style** list, choose **Phosphate**. Click **Apply**.
6. Similarly, select the two bases in the DNA fragment and click **Apply** for the *Base* style.

**Tip** The information about a user-defined style is stored on your local hard drive in the private directory that is specified in the **Preferences** dialog box, **General** tab (on the **Options** menu, click **Preferences**), in a file called USERSTL.SK. If you want to share your Style file with friends and colleagues, ask them to place a copy of your USERSTL.SK into their private directory.

## 11.5 Setting a Default Style

On the **Properties** panel, from the list of styles, choose the required style and click **Set Default** and the selected style becomes the default and any structure drawn from this point on will be of that style.

–OR–

On the **Options** menu, point to **Set Structure Drawing Style** and click the required style on the submenu.

**Note** To set the default, you do not have to save your style. You may just specify the required attributes on the panel tabs, and click **Set Default**. Your attributes will become the default.

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## 12. Working with Styles in Draw Mode

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### 12.1 Objectives

In the Draw mode, a style may include attributes of one or several objects: pen, fill, arrow, font, and paragraph. This will allow you to create different styles for text, fillable objects, arrows, and lines.

In this chapter, you will learn how to:

- Change an object's style
- Save a style
- Set a default style

### 12.2 Changing the Style of an Object

In Chapter 9 which describes how to draw a DNA chain and orbitals, there was a brief introduction to changing an object's style. In this section, we are going to give you a general procedure.

1. Switch to the **Draw** mode.
2. Select the object (or objects) whose style you want to change.
3. Double-click the selection to display the **Objects** panel. Depending on the kind of selected object (shape, linear object, arrow, text, spectrum, table, or structure) the **Object** panel may contain different buttons:



4. Combine your choices from the tabs and their boxes to create your style and click **Apply** to apply changes.



**Note** Settings from the **Common** tab will be applied to all the objects. For example, changing the pen color to red will affect shapes, lines, and structures. If you change any attribute in the **Shapes** tab, it will affect shapes only.

## 12.3 Saving a Style

The style you have created can be saved:

1. To save the specified settings, on the **Objects** panel, click **Save As New Style**.
2. In the **Save User Style** dialog box that appears, select the attribute that should be included in your style. For example, if you want to create a special style for text, make sure that the **Font Style** and **Paragraph Style** check boxes are selected.
3. Type the name for your style and click **OK**. The style will be added to the list of styles and can be then loaded to the **Objects** panel and applied to the selected objects or set as the default.

## 12.4 Applying an Existing Style

You can apply the saved style (either built-in or user-defined) to any selected object.

1. Select the object(s) whose style you want to change.
2. Double-click the selection to open the **Objects** panel.
3. Click **Load** and, from the list of styles, choose the required one. The style attributes will be loaded into the panel.
4. Click **Apply**.

## 12.5 Setting a Default Style

The default style attributes can be specified on special style panels that can be displayed using the commands from the **Tools** menu:

- **Pen Style Panel**
- **Fill Style Panel**
- **Arrow Style Panel**
- **Font Panel**
- **Paragraph Panel**
- **Table Panel**

The style attributes specified on any of these panels immediately become the default.

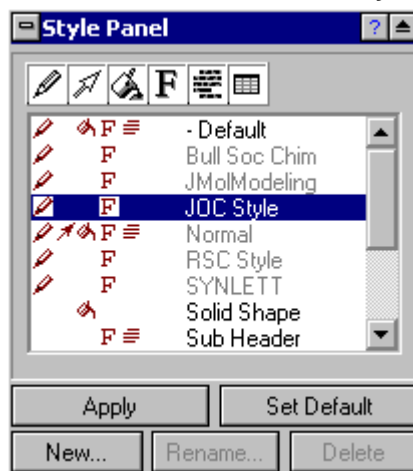
You can load any existing style into any of these panels by clicking **Load**. The style is automatically loaded into all of the style panels and becomes the default.

You can also load style attributes from the drawn object into any of the style panels. Click **Update From**, and then the object. The object's style attributes are loaded into every style panel and are automatically set as the default.







**Note** If you want to change the style of a specific drawn object without effecting the default, use the **Objects** panel (see Section 12.2).

## 12.6 Managing Styles

To manage your styles (save, apply, rename, delete, or set as default), you can use the **Style Panel**. To display this panel, from the **Tools** menu, choose **Style Organizer Panel**:



On this panel, you can do the following:

Desired Action	Button to Click
View the styles that contain a specific attribute (pen, arrows, fill, font, paragraph, table)	Click the appropriate button at the top of the panel.
View the whole list of styles	Click the buttons at the top of the panel so that they all are selected:      .
Apply the style to the selected object(s)	Select the needed style in the list and click <b>Apply</b> .
Set the style as default	Select the needed style in the list and click <b>Set Default</b> .
Create a new style based on the current default settings	Click <b>New</b> .
Rename the style	Select the needed style in the list and click <b>Rename</b> . Note that the built-in styles (they appear in gray in the list) cannot be renamed.
Delete the style	Select the style in the list and click <b>Delete</b>  . Note that the built-in styles (appearing in gray in the list) cannot be deleted.

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## 13. Creating Report Templates

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### 13.1 Objectives

ACD/Report Template is a special tool that is used to create a template and generate standard reports on its basis instead of repeating the same editing procedure for each report. Currently, you can do this in ACD/ChemSketch. ACD/ChemSketch allows you to create report templates for data supported by 1D NMR, 2D NMR, MASS, UV-IR, CURVE, and CHROM modules of ACD/SpecManager. Later, we are going to enlarge the list of programs which allow the creation template-based reports. With the **Report Template** tool it is easy to meet your corporate standards.

Using ACD/Report Template, you can arrange multiple ACD/SpecManager objects (such as tables, graphs, parameters, structures, and others) belonging to one or several spectra/curves/chromatograms on one or several pages.

If you do not have any of the mentioned above modules, skip this chapter.

In this chapter, you will learn how to:

- Enter the Report Template mode
- Evaluate the information that will be inserted into the report, and decide which objects should be included
- Insert objects into the template
- Assign properties to each object
- Arrange the objects in an acceptable manner
- Save the template to a separate file

### 13.2 About Report Templates

Each report template consists of so called **TEMPLATE OBJECTS**, or just **OBJECTS**, each assigned to a certain SpecManager item (spectrum as such, table, chemical structure...) or other items (text label) and having certain properties which regulate the display of these items. For the most part, these properties are correlated with SpecManager properties for the corresponding module. If template objects have different identification numbers or **IDs**, they refer to different SpecManager documents. If there are no IDs assigned, all objects in this template refer to the same SpecManager document.


It is possible to insert your company logo into template-based reports as a bitmap (on how to insert a bitmap, see the corresponding topic in Report Template Help).

Moreover, as soon as the template-based report is ready, you can easily insert all proper amendments using standard ChemSketch Object panels which appear immediately by double-clicking.

**Report Template** can be accessed via the **Report Template** button  on the **Drawing** toolbar (**Draw** mode).

### 13.3 Entering the Report Template Mode

Many ACD/Labs applications allow you to create reports according to templates. However, to create a template, you need to use to ACD/ChemSketch, which is offered free of charge and thus available for all ACD/Labs customers.

1. Switch to the **Draw** mode.
2. Click **Report Template**  on the leftmost toolbar. Note that the informative cursor appears.

There exists a vast amount of information that you can insert into a report template. To get the first insight into report templates, let's create an example.

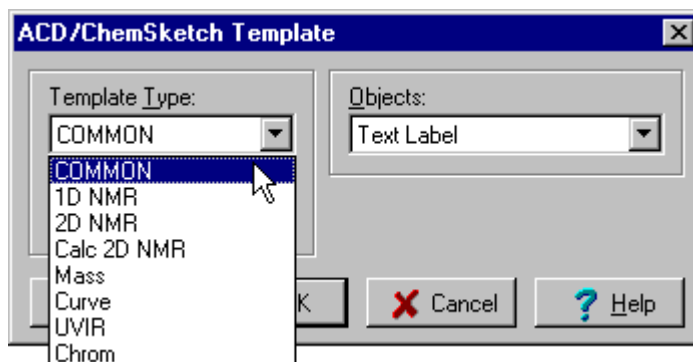
### 13.4 Inserting Template Objects

1. With the Report Template mode on, point to the top left corner of the working area and drag to define the size of the first template object.



**Note** Do not worry too much about the size of the template box at this stage because you can change the size of the template box later.

2. As soon as you release the mouse button, the **ACD/ChemSketch Template** dialog box appears. The **Template Type** list contains all of the SpecManager modules that are installed on your computer, as well as the **COMMON** type (selected by default). Depending on the template type selected, the **Objects** list looks different.



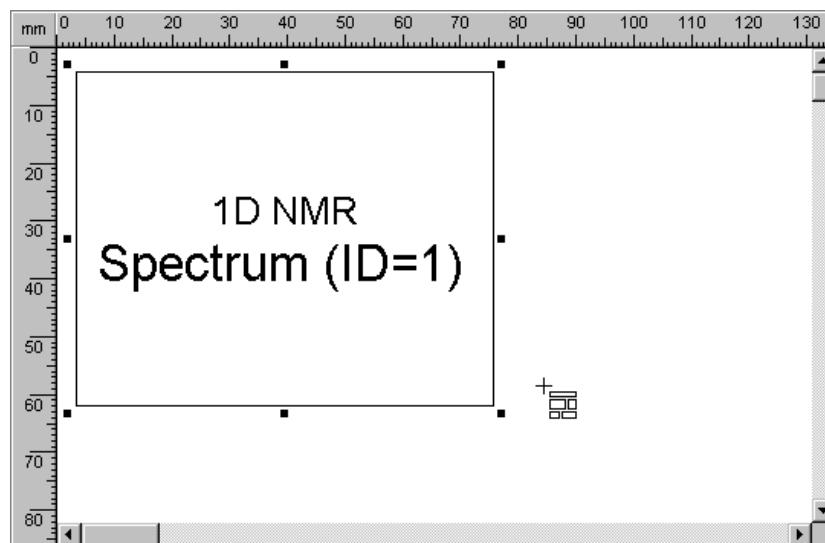
**Note** When you select different template types in the list, the notice in the template box in the ChemSketch workspace is changed correspondingly to let you know what kind of template you are creating.

3. Now, we are going to create a template for 1DNMR and 2DNMR modules. However, if you do not have these modules of SpecManager, select other template types instead. In the

**Template Type** list, select **1D NMR**, and then in the **Objects** list, click **Spectrum**. Note that the object in the workspace changes accordingly. In the **ID** box, type or select "1" to refer this object to a spectral document with the same ID.

**Note** On how to assign IDs to SpecManager documents, see the corresponding Report Template Help topic: *How to create a template based report*. Report Template Help is a part of both ChemSketch Help and SpecManager Help.

4. In the **ACD/ChemSketch Template** dialog box, click **OK**. The dialog box disappears but the Report Template mode is still active.

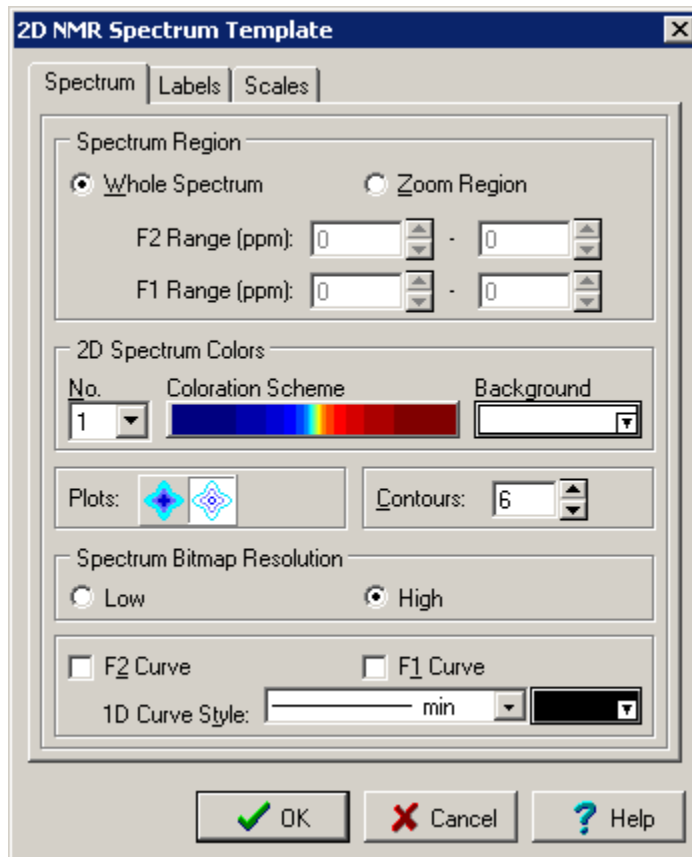



5. Drag in the workspace to the right of the first object to draw a second template object approximately of the same size. The ChemSketch Template dialog box immediately pops up.
6. In the **Template Type** list, click **2DNMR**, and then, in the **Objects** list, select **Spectrum**. Thereby, we have allocated a spot for 2DNMR spectrum. As this spectrum will be in another spectral document, we need to assign it a different ID. Type or select "2" in the **ID** box.

**Note** If you have one module of SpecManager in your possession, and therefore, one module related type, insert a spectrum/chromatogram/curve (later on, spectrum) of the same type twice but assign different IDs to them. When creating a report according to this template, you will be able to insert two different spectra of the same type.

## 13.5 Setting Display Preferences

1. Click **Settings**  to set the spectrum display parameters for the 2D NMR spectrum.




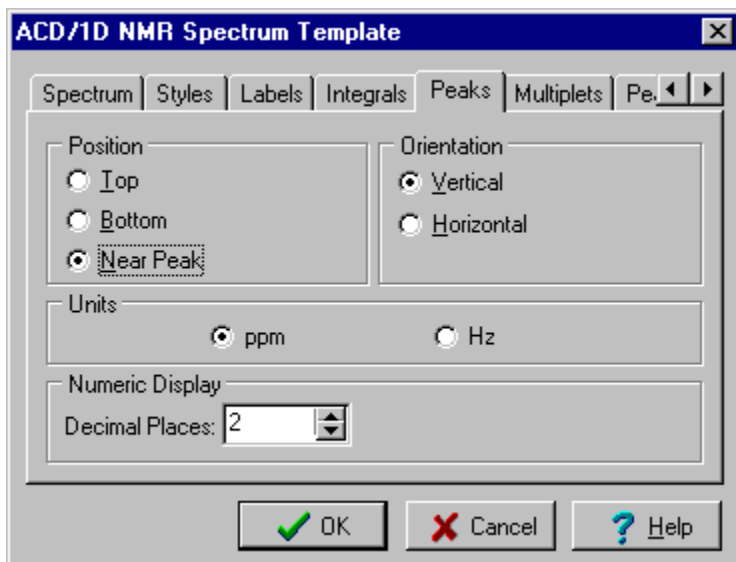
**Note** Each time you click **Settings**  in the **ChemSketch Template** dialog box, a dialog box corresponding to the currently active **TEMPLATE OBJECT** appears. Each **TEMPLATE OBJECT** has its inherent set of options included into the corresponding dialog box. If you open the **Spectrum Template** dialog box for a different module, it will naturally look different. However, all these dialog boxes contain the same options as the **Preferences** dialog boxes in the corresponding module. To get more information on the options available, click **Help**.

2. Now, we are going to set the display preferences which are common for the majority of modules. In the **Spectrum Region** area, click **Whole Spectrum**. In this case, the entire spectrum will be inserted into reports made according to this template.

**Note** If you select **Spectrum Region**, only a zoom region will be inserted.

3. Switch to the **Labels** and **Scales** tabs and, if necessary, change the settings for these elements.
4. Click **OK** to apply changes.
5. In the **ACD/ChemSketch Template** dialog box, click **OK**. The dialog box disappears but the Report Template mode is still on and the second template object (2D NMR Spectrum (ID=2)) remains selected (has black nodes around it).

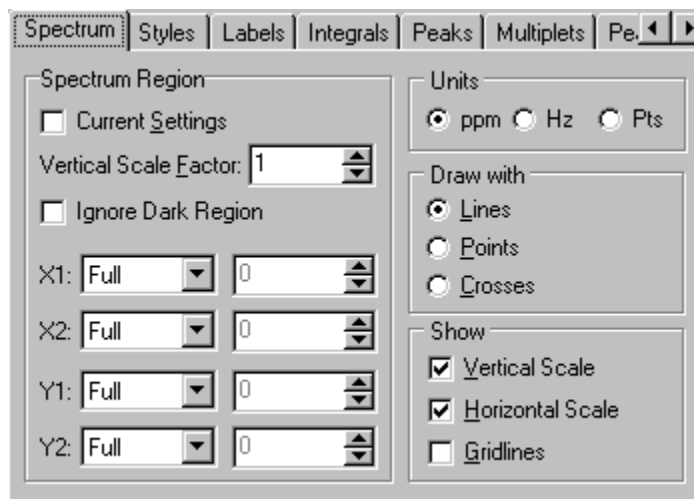
- Double-click the first inserted template object to make it active and to display the **ACD/ChemSketch Template** dialog box. Make sure that in the **Objects** list, the **Spectrum** option is selected and click **Settings**  to customize the preferences for the display of the 1D NMR spectrum. The **1DNMR Spectrum Template** dialog box appears.
- Click the **Peaks** tab:




- Specify the display of the peak labels: in the **Position** area, click **Near Peak**, and in the **Orientation** area, click **Vertical**. In the **Numeric Display** area, type or select "2"—in this case, two decimal places will be displayed in peak labels.

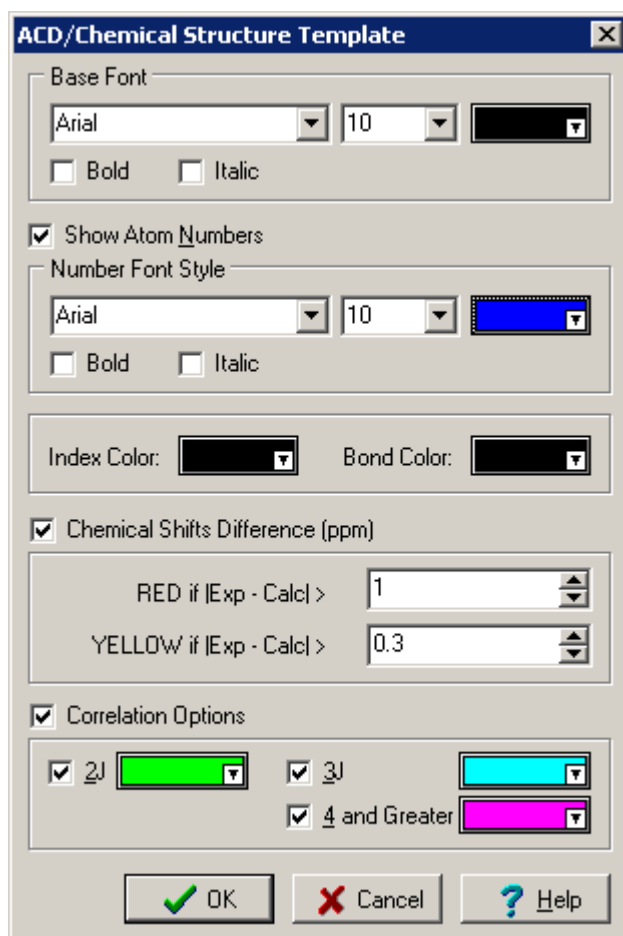
**Important** If no peaks have been picked on a spectrum inserted into a future template-based report, they will naturally not be visible on the spectrum. This is also true for other options (integrals, multiplets, curves...).


- Click the **Spectrum** tab. In the **Spectrum Region** area, set the X1, X2, Y1, and Y2 options to **Full**, and in the **Show** area, select the **Vertical Scale** and **Horizontal Scale** check boxes.



**Note** Although, when setting display preferences, you do not see any immediate outcome, the settings are stored by the program and placed into the corresponding template object.

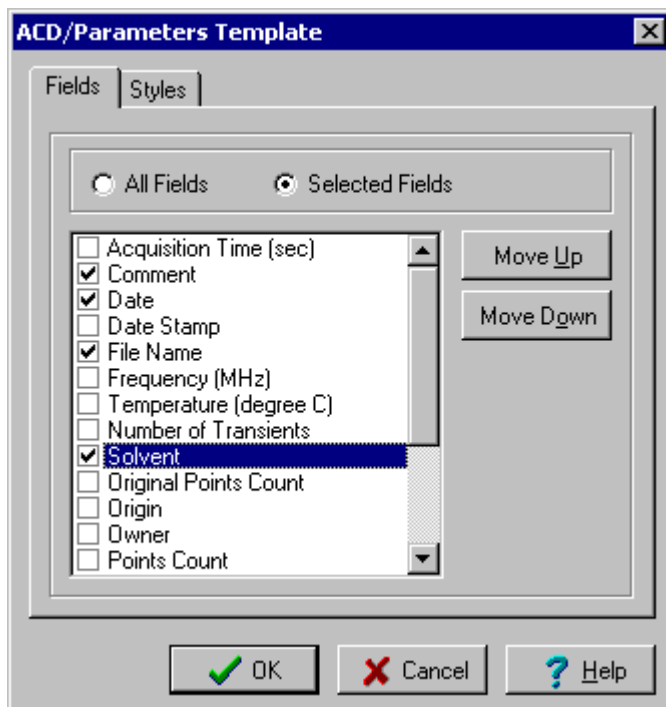
10. Look through the tabs in your module-related dialog boxes to find out what other options are available. To get more detail, click **Help**. If required, set other options. Click **OK** to apply changes.
11. In the **ACD/ChemSketch Template** dialog box, click **OK** to close it.
12. Select the **Report Template** tool and for the **1D NMR** template type, insert a **Chemical Structure** object with **ID=1** (for help, use the instructions listed in Section 13.4). When in the ACD/ChemSketch Template dialog box, click **Settings**  to customize the display of the structure:

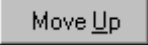



13. In the **Base Font** area, set preferences for font style, size, and the color that will be used to draw the structure. Click the **Bond Color** box to display the color palette, and then select the color for bond display. Select the **Show Atom Numbers** check box, and then set the proper font style for atom numbers under **Number Font Style**. Close both dialog boxes by clicking **OK**.
14. Now, insert one more object of the **1DNMR** type—**Spectrum Parameters** with **ID=1**. To customize the display of the spectrum parameters in reports, click **Settings** .

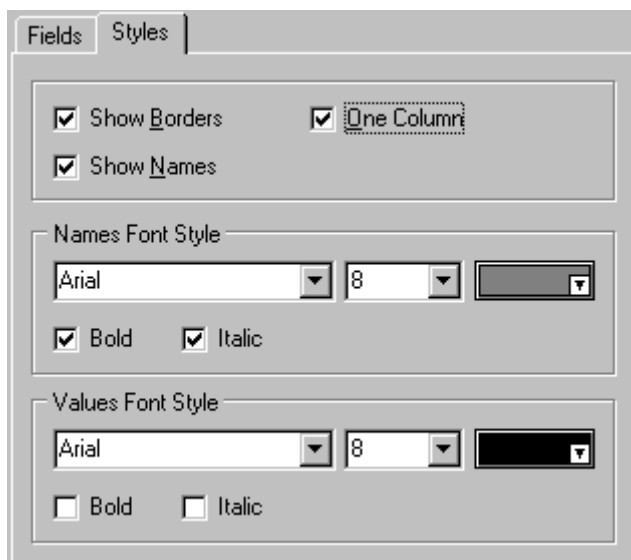




15. The **Fields** tab of the **Parameters Template** dialog box allows you to select those spectrum parameters which you would like to appear in reports made according to this template and to tune in the display order of the selected parameters. Select the **Select Fields** option at the top of the dialog box, and then clear all check boxes except for *Comment*, *Date*, *File Name*, and *Solvent*. The fields that remain selected will be inserted into the report.

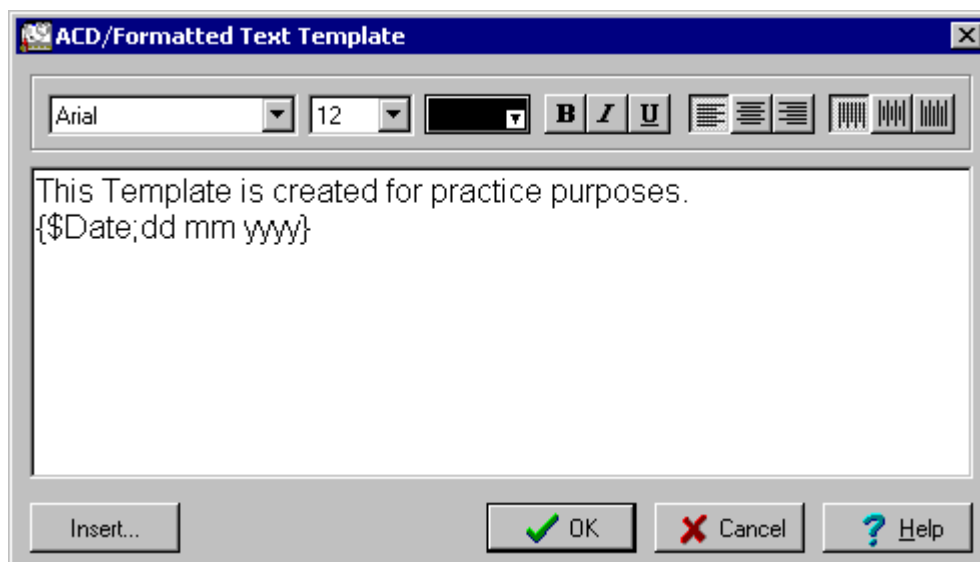




**Note** You can use the **Move Up**  and **Move Down**  buttons to rearrange the fields order.

16. Click the **Styles** tab. Select the **Show Borders** check box to show horizontal and vertical borders between each Name-Value pair. Select the **Show Names** check box to show the field names, otherwise only the values will be displayed. Select the **One Column** check box to show parameters in a column: one Name-Value pair under another:

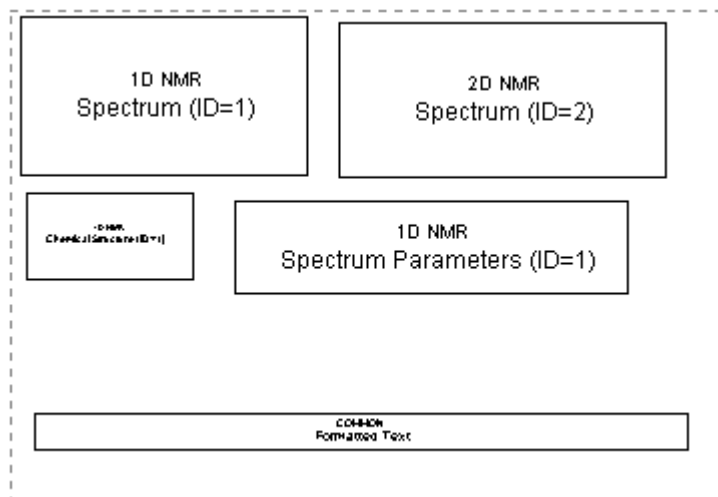


17. Click **OK** in both dialog boxes.
18. Now we are going to add a subscription. Make sure that the **Report Template** tool is on and using the instructions listed in Section 13.4 above, insert a long narrow box along the bottom border of the template. In the **ACD/ChemSketch Template** dialog box that appears, select **COMMON** in the **Template Type** list, and in the **Objects** list, click **Formatted Text**. Click **Settings** .
19. The **Formatted Text Template** dialog box appears. Using this dialog box, you can add any textual information to the template which will appear in any report made according to this template. Type a few words to characterize the series of reports you are going to create on the basis of this template, for example "*This Template is created for practice purposes*", and then click the **Insert** button  that allows you to automatically insert current date, time, page number, or any other user defined label. In the **Select Field** dialog box, select **Date** in the **Name** list, and then click **OK**. Set font and alignment preferences.





**Note** **Alignment** buttons located in the top right-hand corner of the **Formatted Text Template** dialog box allow you to tune the horizontal alignment of the text  (over the left border, between the borders, and over the right border respectively), and the vertical alignment  (over the top border, between the borders, over the bottom border). *Border* here denotes the **template object** border.

Now, your ChemSketch working area should look something like this:




## 13.6 Arranging Template Objects

After all of the template objects have been inserted, it may be necessary to resize and rearrange them so that they fit properly.

1. Switch to the **Select/Move/Resize** tool .
2. Select the object you want to move or resize.
3. Point to the inside of the template object and the **Move** pointer  appears. Now, you can relocate the object by dragging it.
4. Point to any node and the corresponding **Resize** pointer appears. Now, you can resize the objects by dragging it.
5. Using the above instructions, resize and rearrange the template objects to suit your requirements.

## 13.7 Saving and Applying Report Templates

As soon as a template is ready, you need to save it into an \*.SK2 file, otherwise, you will not be able to use it later.

1. From the **File** menu, choose **Save As** to display the **Save Document As** dialog box, and then select the name and location for the file.
2. Switch to the Processor window.
3. Open the documents you want to base your report on, and then from the **Edit** menu, point to **Create Report**, and choose **by Template**; from the **Edit** menu, point to **Export Report to PDF**, and choose **By Template**; or from the **File** menu, point to **Print Report**, and choose **By Template** or click the corresponding buttons .
4. In the **Select Report Template** dialog box that appears, select the location and file name of your saved template.
5. After the report is created, you are automatically transferred to the ChemSketch window. If necessary, edit the report by double-clicking the objects that open the **Objects** panels.

For further detail on creating template-based reports, see the User Guides on the corresponding modules of SpecManager or look through the corresponding **SpecManager Help** topics.

**Tip** If you want to try the template before saving it, take a look at the ChemSketch title bar to find out the name that ChemSketch has given to the current template (noname00, 01, 02, etc.). Switch to the Processor window by clicking the Processor button on the **Window Switching** bar. When in SpecManager, open (a) spectral document(s), and then follow the above steps to open the **Select Report Template** dialog box where you can enter the template file name given by ChemSketch.