ACD/ChemSketch

Version 2012 for Microsoft Windows

Tutorial

Drawing Chemical Structures and Graphical Images

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Before You Begin

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 a freeware at our Web site:

http://www.acdlabs.com/resources/freeware/chemsketch/

> **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 the freeware and also the Frequently Asked Questions (FAQs) can be found on our Web site at:

http://www.acdlabs.com/resources/knowledgebase/faqs/chemsketch_freeware.php.

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 to the Windows Classic Theme (with dismissed gradients) of the operating system’s Display Properties.

This tutorial is provided in electronic form, readable with Adobe 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*** means point to an item, and quickly press and release the left mouse button.
- ***Right-click*** means point to an item, and quickly press and release the right mouse button.
- ***Double-click*** means point to an item, and quickly press and release 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 either by 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. We offer free ACD/ChemSketch, an ACD/Log*P* 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). The movies can be run from the ACD/Labs software folder, \\MOVIES.

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 site.

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 page:

http://www.acdlabs.com/newsletters/

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://www.acdlabs.com/support

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

Updates of our Desktop and Enterprise products are made throughout the year. These intermediate releases (bringing the actual version number of a program, for example, from *N*.00 to *N*.01) often contain new functionality along with additional bug fixes and support for new file formats. To check if there is a new update available and to have this sent to you, please contact your local agent or our Technical Support Department. Before calling, we recommend that you have ready the name of the software purchaser, the product name, version number, build number, and license ID of the product you are contacting us about. All Desktop 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. For more information, refer to the *ACD/Updater User's Guide* located in the ACD/Labs documentation folder, \\DOCS\UP_CLNT.PDF.

1. Basics of ACD/ChemSketch

1.1 Objectives

This chapter will familiarize you with:

- Starting ChemSketch;
- Setting and changing file associations;
- Setting default directories; and
- Quitting the program.

Information about minimum system requirements as well as installation instructions are provided in the Quick Installation Guide booklet which is included in every shipment of ACD/Labs software.

1.2 Starting ACD/ChemSketch

Once ACD/ChemSketch has been installed on your computer, use one of the following ways to start it:

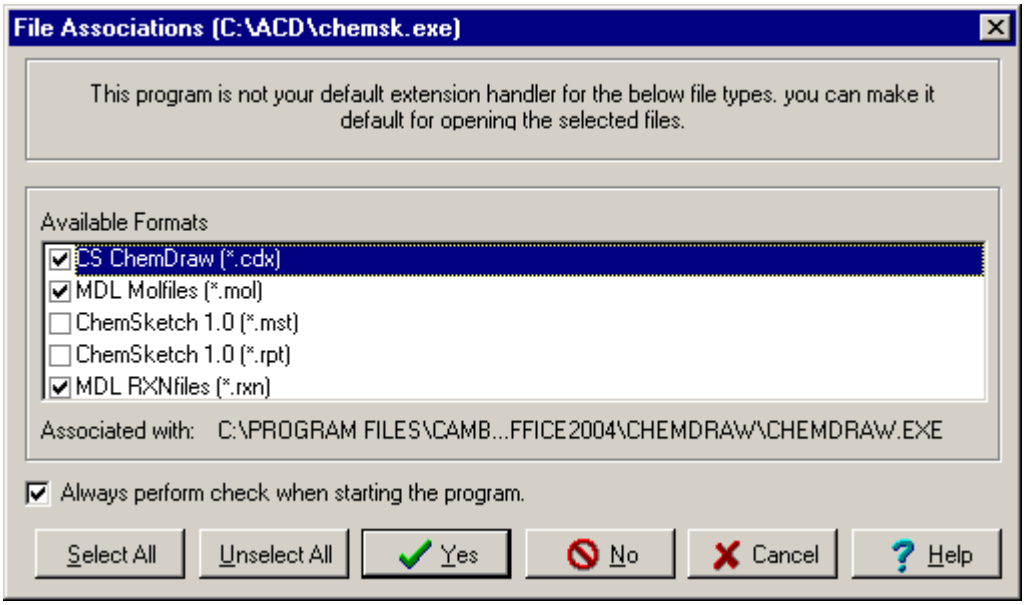
- On the **Start** menu, point to (**All**) **Programs**, after that to **ACDLABS 2012.0**, and then choose **ChemSketch**; or
- In the folder where the ACD/Labs software is installed (by default, this is \\ACD2012), double-click the CHEMSK.EXE program file; or
- If you have other ACD/Labs programs running, from the **ACD/Labs** menu of the program, choose **ChemSketch**.

> **Note** If you have created a shortcut to ACD/ChemSketch on the Windows desktop, click it to run the program.

As a result, you should see an ACD/ChemSketch 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), MDL 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.

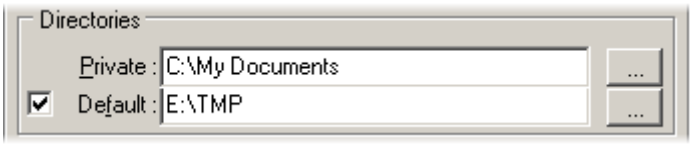
3. Set the application that should be used to open the file and select the **Always use this program** check box.
4. Click **OK** and close Windows Explorer.

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 (TEMPLATE.CFG and QRSTYLES.STL files).

3. Click **OK**.

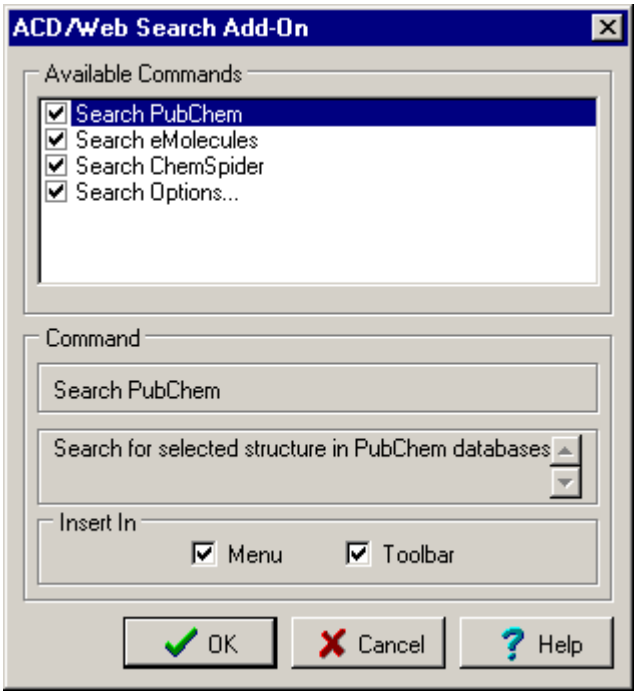
1.5 Installing Add-Ons

Starting from version 8.0, ACD/Labs applications support 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 an add-on in ACD/ChemSketch, 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 ACD/ChemSketch interface.
5. In the **Insert In** area, choose where the add-on commands should be added: as commands to the **Add-Ons** menu and/or as buttons to the General toolbar (if it was implemented by the add-on author), and click **OK**.
6. Click **OK** in the **Add-on Organizer** dialog box, and ensure that the menus and/or buttons are added to the interface.

1.6 Quitting ACD/ChemSketch

The ChemSketch window can be opened when you start either CHEMSK.EXE or almost any of the ACD/Labs applications (except for ACD/Labs Batch programs). So, when you quit an ACD/Labs application, ACD/ChemSketch will be quitted correspondingly.

You can quit ACD/Labs programs in any of the following ways:

- On the title bar of any window, click **Close** ;
- Press either ALT+X or ALT+F4—*depending on a specific ACD/Labs application*;
- From the **File** menu, choose **Exit**—*these three ways will close only the specific ACD/Labs application to which ACD/ChemSketch serves as a drawing module (or ACD/ChemSketch itself in case CHEMSK.EXE has been run on its own account)*; or
- From the **ACD/Labs** menu, choose **Exit All**—*this command will attempt to close all ACD/Labs programs that are currently open, one by one.*

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

> **Note** To continue with this tutorial, do not quit ACD/ChemSketch.

2. Drawing Simple Structures

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 various atoms, bonds, as well as labels and polymers;
- Flip a drawn molecular structure;
- Select, rotate, and resize drawn structures;
- Output the structure to a file, document, or printer; and
- Clean the screen.

2.2 Drawing Atoms, Bonds, and Labels

Drawing chemical bonds and atoms is the basic activity in ACD/ChemSketch. Before you start drawing, make sure that you are in the Structure mode which is applicable for all of the actions described in the sections that follow:

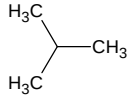
- On the General toolbar, click **Structure** 

.

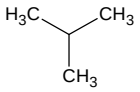
2.2.1 Using the Draw Normal Tool

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.

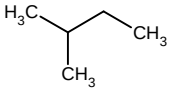
1. Make sure that the **Draw Normal** tool  is enabled on the Structure toolbar and that the **Carbon** button  is selected on the Atoms toolbar.
2. Click in an empty space to draw *methane* CH_4.
3. Point to CH_4 to select it (you will see a rectangle around the methane formula), and then click it to add a methyl group to it while creating *ethane* CH_3—CH_3.
4. Click twice the same carbon to draw *2-methylpropane*:



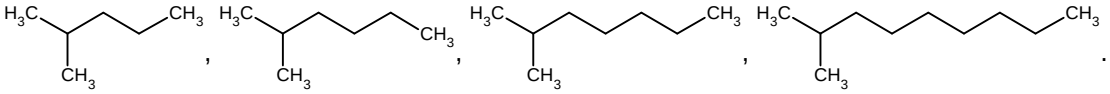
5. On the Structure toolbar, click **Set Bond Vertically**  , and click the lower bond of the structure to rotate it to this orientation:



6. On the Structure toolbar, click **Draw Normal**  .
7. Click the right-most carbon atom to draw *2-methylbutane*:



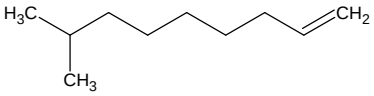
8. Repeat the above step to draw the following homologous structures:



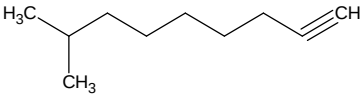
2.2.2 Drawing Double and Triple Bonds

Now we are going to draw double and triple bonds:

1. On the *2-methylnonane* structure, point to the last drawn bond (you will see a rectangle around the bond), and then click it to make a double bond:



2. Click there again to make a triple bond:



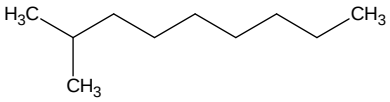
2.2.3 Cancelling Actions

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**  one more time to return to the *2-methylnonane* structure:

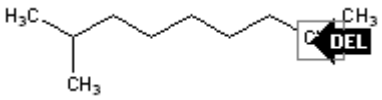


> **Note** The **Undo** command can be repeated up to 50 times. When you begin to draw more complex structures or graphical objects, we recommend that you develop a habit of saving your work to a file after making several changes.

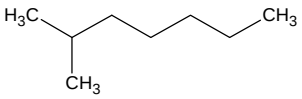
2.2.4 Deleting Individual Atoms

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 last but one carbon atom of the main chain as shown on the picture:



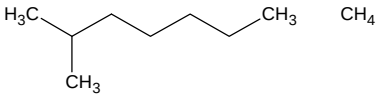
The structure now looks like this:



Note that the whole ethyl group is removed from the *2-methylnonane* structure.

> **Note** Such a simultaneous deletion of terminal group is actual for the CH_3, SiH_3, NO_2, *etc*. groups with non explicitly drawn substituent atoms.

3. Now, click **Undo**  to reverse the changes.
4. Holding down CTRL, click the same carbon atom again:



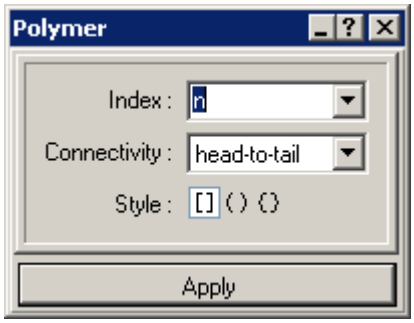
As you can see, the last but one atom is removed while the terminal atom of the main chain attached to the deleted one is now retained on the page.

5. Click **Undo**  to reverse the changes and return to the *2-methylnonane* structure.

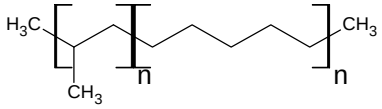
2.2.5 Polymers

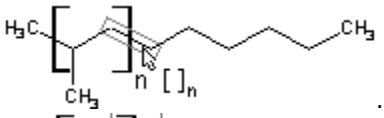
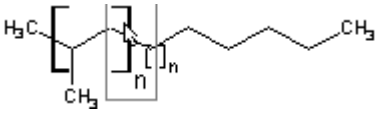
ACD/ChemSketch allows you to draw polymeric structures:

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

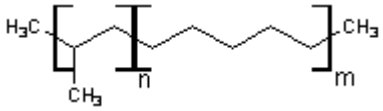


2. Select two areas to be turned into different monomeric units of a polymer as shown below either by clicking starting and ending bonds or by dragging over the required parts of the structure. As soon as the area is selected, the polymer appears in the workspace:



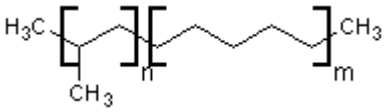
> **Tip** When drawing the second monomeric unit, first point to the bond (not to the bracket) and click.
>
> Right cursor position:
>
> 
>
> Wrong cursor position:
>
> 

3. With the second monomer unit selected, in the **Index** box of the **Polymer** panel, enter different unit's index, e.g., *m*, and then click **Apply**. The structure now looks as follows:



4. Leave the Polymer Drawing mode by closing this panel.

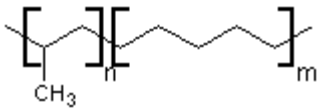
5. On the Structure toolbar, click **Select/Move**  , and then select and move adjacent brackets of the monomeric units apart from each other:



2.2.6 Pseudo Atoms

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

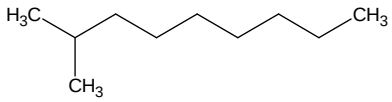
1. On the Atoms toolbar, click the lower right triangle of the **Radical Label** button  , and then, from the **Radical Labels** menu, choose **Pseudo Atom**  .
2. Click terminal atoms of the structure to replace them with blank atoms and get an open-ended polymer structure:



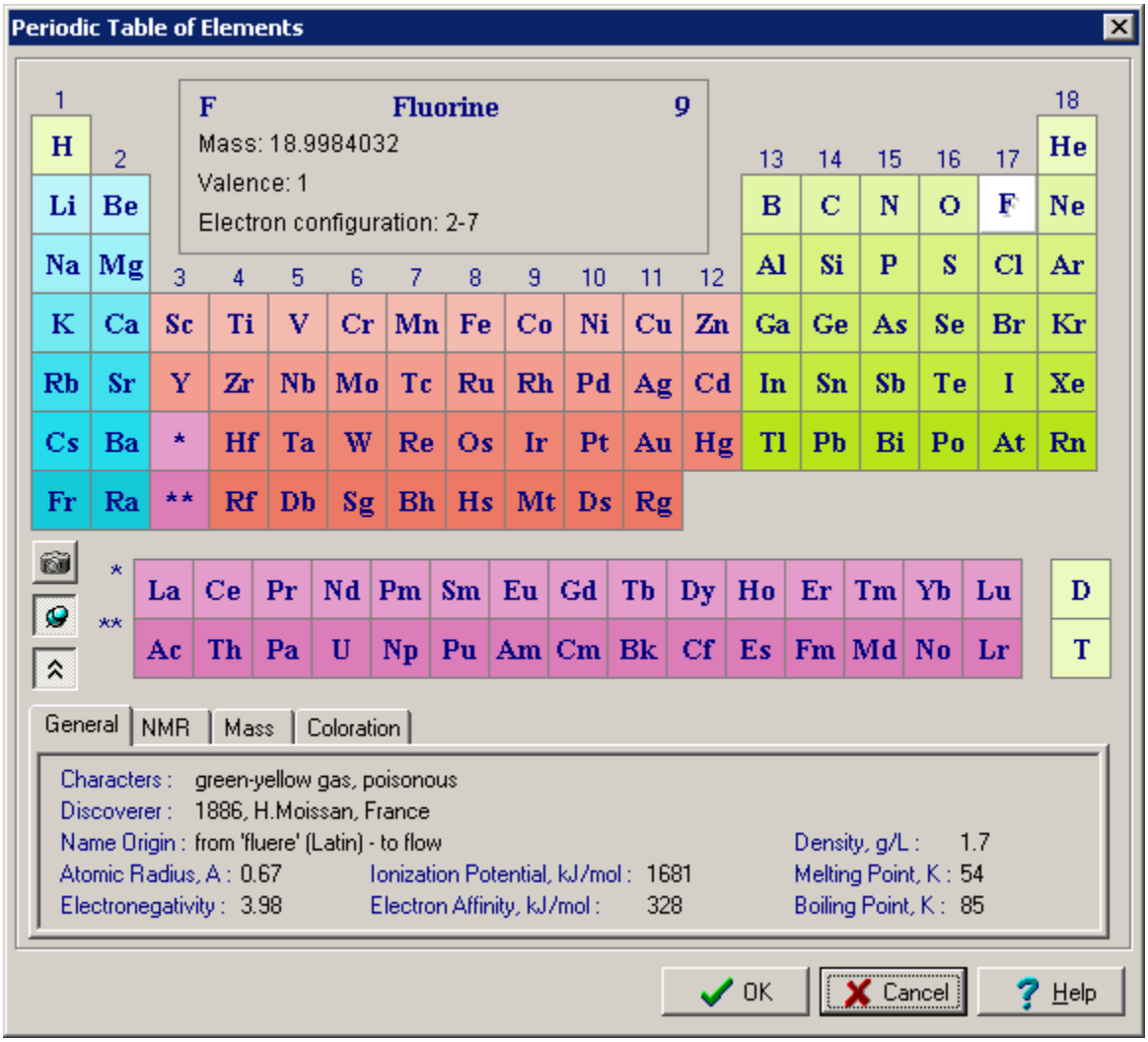
2.2.7 Changing the Atom

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 *2-methylnonane* structure, or draw it anew:

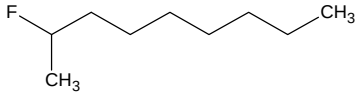


2. On the Atoms toolbar, click **Periodic Table**  to display the **Periodic Table of Elements** dialog box:



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

4. Click the leftmost carbon atom to replace it with a fluorine one:



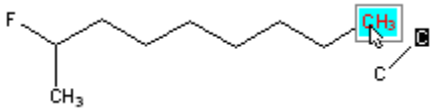
> **Note** When you select user-defined elements from the Periodic Table of Elements, the corresponding buttons are automatically added to the Atoms toolbar. To remove these buttons from the Atoms toolbar, double-click the Atoms toolbar and in the message box that appears, click **Yes**. This will remove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

2.2.8 Using the Draw Continuous Tool

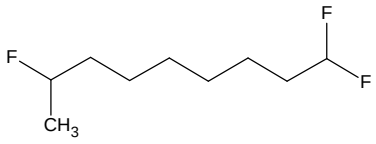
This mode is very convenient for “sprouting” new atoms from a selected atom.

> **Note** When the mode is active, bonds can only be drawn from the highlighted atom.

1. On the Structure toolbar, click **Draw Continuous**  . Alternatively, you can press the right mouse button to switch to this drawing mode.
2. Ensure that the **Fluorine** button  is still selected on the Atoms toolbar.
3. Click the rightmost carbon atom in the drawn structure to highlight it:



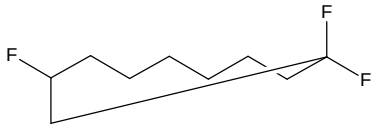
4. Click again to sprout fluorine from the selected carbon atom.
5. Repeat Steps 3-4 for the same carbon atom again to sprout up the second fluorine atom:



2.2.9 Drawing Bond Between Two Atoms

When either **Draw Normal**  or **Draw Continuous**  drawing tool is selected, dragging from one atom to another draws a single bond between them:

- With one of the drawing tools active, point to one of the terminal carbons and drag to another terminal carbon to draw the following structure:

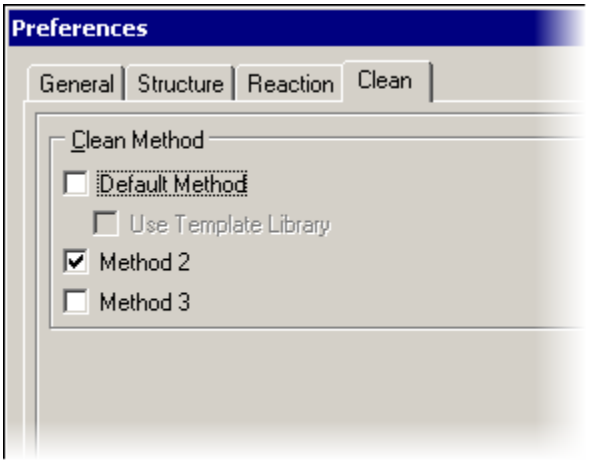


> **Note** If you drag to or from an empty space, a new atom is inserted at the beginning or the end of the drawn bond instead.

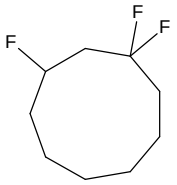
2.2.10 "Cleaning" Structure

To standardize all the bond lengths and angles in the drawn structure ("clean" the structure), follow the steps:

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

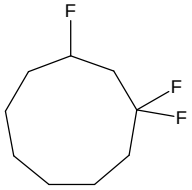


2. Click **OK** to close the dialog box.
3. On the Structure toolbar, click **Clean Structure**  :



> **Note** 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^o angles and the bonds near the sp carbon at 180^o (linear). If you draw geometrical and stereoisomers, the **Clean** command standardizes their bond lengths and angles while retaining all of their structural significance.

4. On the Structure toolbar, click **Set Bond Vertically**  , and click the carbon-fluorine bond of the structure to rotate it as follows:

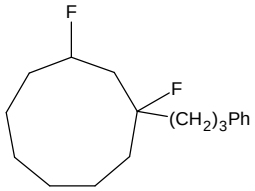


2.2.11 Editing Atom Labels

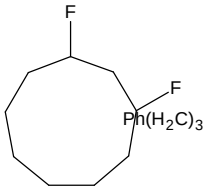
The **Edit Atom Label** tool allows you to substitute terminal atoms with shorthand abbreviations.

Using the structure cleaned in the previous section, follow the steps below:

1. On the Atoms toolbar, click **Edit Atom Label**, and then click the lowermost fluorine atom on the drawn structure.
2. In the **Edit Label** dialog box that appears, type **(CH2)3Ph**, and click **Insert** Insert. Note that the label is inserted in the desired position and the indexes are automatically subscripted:

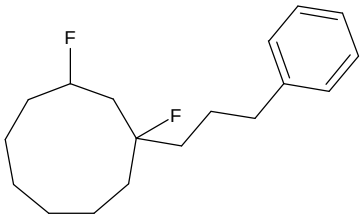


3. Click **Change Position**, and then click the label to invert it:



> **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 resulted shorthand abbreviation to open the **Edit Label** dialog box again. Then click **Expand** Expand to obtain the following structure:



> **Important** Only group abbreviations that substitute terminal atoms as atom labels can be expanded by using the **Expand** Expand tool.

2.2.12 Rotating Structural Fragments

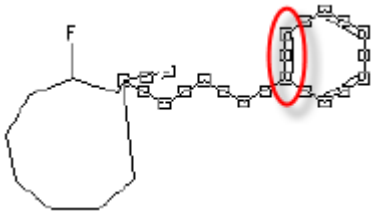
The expanded 3-phenylpropyl label of the drawn structure looks not smooth enough, so we will try to improve its appearance by sequential using of drawing tools of ACD/ChemSketch.

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

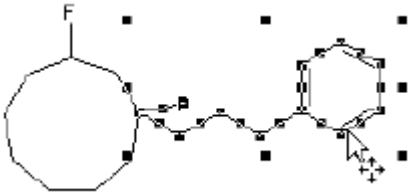
> **Note** There are two selection modes in ACD/ChemSketch: the first mode () selects objects with the rectangular selection box, while the second mode () selects objects with the lasso selector line. The latter one, the lasso, allows you to select objects in a more specific and precise manner.

2. Drag over the structure to select the following fragment:

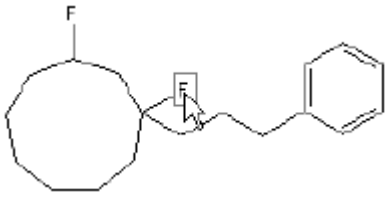
3. On the Structure toolbar, click **Set Bond Vertically**  , and then click the following bond in benzene to rotate the entire fragment:



4. On the Structure toolbar, click **Select/Move**  , and then move the selected fragment to the appropriate position:



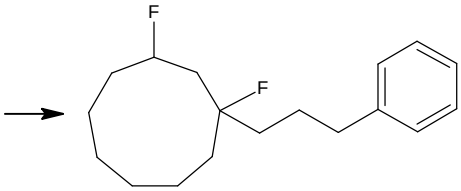
5. Click outside the selection to cancel it, and then drag up the fluorine atom of the fragment as follows:



2.2.13 Drawing Chains

Using the **Draw Chains** tool, you can easily draw chains of any length by click-and-drag method.

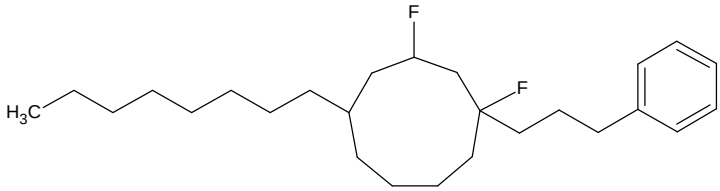
1. On the Structure toolbar, click **Draw Chains**, and point to the atom indicated by the arrow:



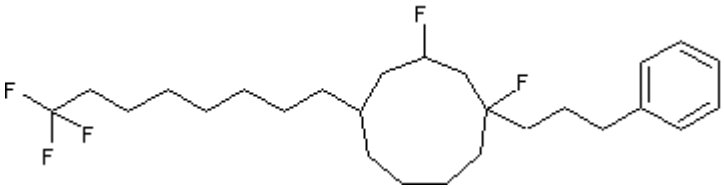
2. Hold down SHIFT and drag left to create a carbon chain and note that the carbon counter (C #) located beside the mouse arrow changes with each carbon added (when dragging forth) or removed (when dragging back).

> **Tip** The dragging draws a chain where the bonds are set at an angle of 120° to each other. However, holding down CTRL while dragging produces a chain where the bonds are set at an angle of 180° to each other.

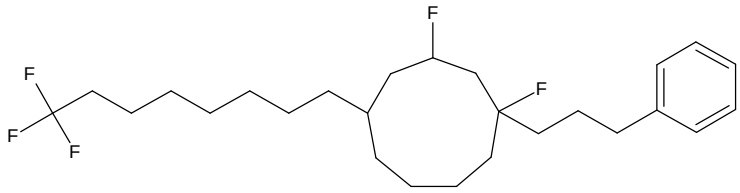
3. Continue the dragging until the counter reaches C 8, then release the mouse button to finish the chain:



4. With the **Draw Chains** tool still active, on the Atoms toolbar, click **Fluorine** F, and then click the leftmost methyl group three times to sprout three fluorine atoms:



5. On the Structure toolbar, click **Select/Move**, then select these three fluorine atoms' bonds, and click **Clean Structure**. The resulted structure of *1,3-difluoro-1-(3-phenylpropyl)-5-(8,8,8-trifluorooctyl)cyclononane* becomes as follows:



> **Note** The CHAPTER2.SK2 file (Page 1/2) with this structure can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons: , Page 2/2, and on the Status bar.

2.3 Cleaning the Screen

If you want to clean the screen in order to draw your structures from scratch, use one of the following ways:

To insert a new blank ACD/ChemSketch document

- On the General toolbar, click **New Document**; or
- From the **File** menu, choose **New**.

To insert a new blank page within current ACD/ChemSketch document

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

To clean up an active page within current ACD/ChemSketch document

- From the **Edit** menu, choose **Select All**, and then, from the **Edit** menu, choose **Delete**; or
- Press CTRL+A to select all the objects on the page, and then press DELETE; or
- On the General toolbar, click **Delete**, click an empty space away from the drawn structures to select all of them, and then click the selection.

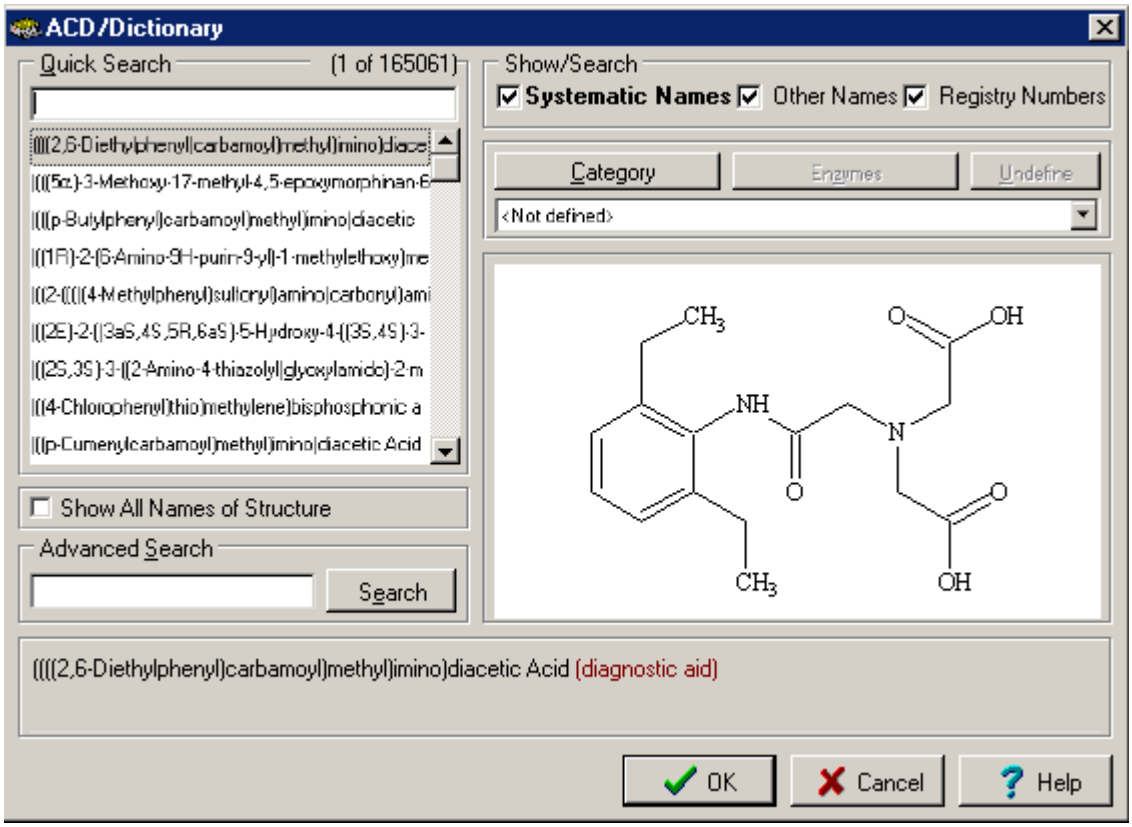
Prior to perform the next actions, clean the screen by inserting second page within current ACD/ChemSketch document.

2.4 Using ACD/Dictionary

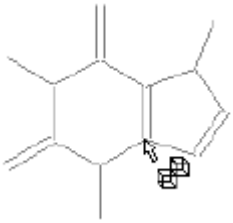
For Commercial Version only

ACD/Dictionary allows you to find a molecular structure for common drug names.

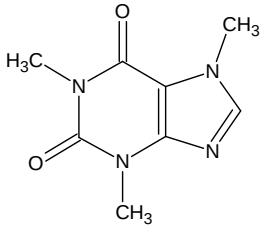
1. On the References toolbar, click **ACD/Dictionary**  to display the **ACD/Dictionary** dialog box:



2. Click the program icon () on the left side of the title bar to view the commands controlling the dialog box, and ensure that the **Copy Structure with Name** command is not selected.
3. In the **Quick Search** box, type *caffeine*. As you type, the list scrolls, displaying 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. Click **OK** to place the selected compound onto the workspace. Note that the structure's outline is attached to the mouse pointer:



5. Move the mouse pointer to an appropriate position on the blank ACD/ChemSketch page created in the previous section, and click to insert the structure:

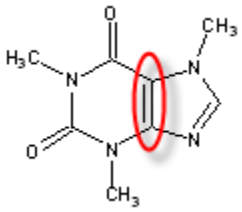


> **Note** For more details on the ACD/Dictionary options, refer to the *ACD/Dictionary User's Guide* located in the ACD/Labs documentation folder (\\DOCS\DICT.PDF).

2.5 Flipping Structures

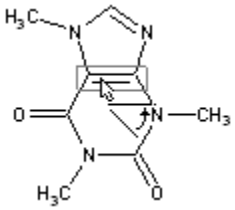
You can rotate or flip the entire structure with a single button click using a set of tools on the Structure toolbar.

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:

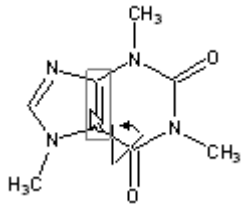


2. On the Structure toolbar, click **Set Bond Horizontally**  , and then click the bond to set it horizontally, rotating the rest of the structure correspondingly:

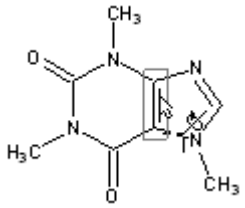
> **Note** Repetitive clicking the bond with this tool will rotate it around the clicked bond.



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



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

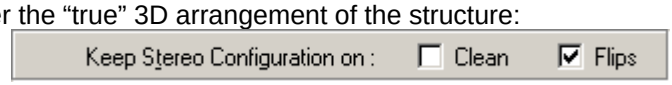
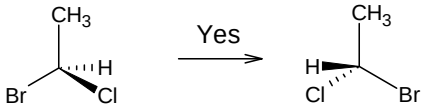
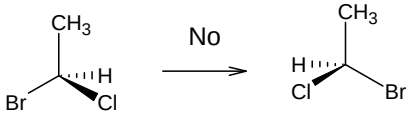


> **Note** The CHAPTER2.SK2 file (Page 2/2) with this structure can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

5. Select the entire structure (or any fragment).

6. On the Structure toolbar, click **Flip Top to Bottom**  , and the selected structure or fragment (or if nothing is selected, then all of the structures drawn in the workspace) will rotate upside-down.

7. Similarly, click **Flip Left to Right**  to flip the selected structure or fragment (or, if nothing is selected, then all of the structures drawn in the workspace) from left to right.

> **Note** Applying the Flip tools may 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:
>
> 
>
>
> 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 (for more information, refer to the *ACD/I-Lab User's Guide* located in the ACD/Labs documentation folder, \\DOCS\ILAB.PDF).

2.6.1 Saving ACD/ChemSketch Document to ChemSketch (.SK2) File

Let us save the entire ACD/ChemSketch document with the structures created in previous sections in the default proprietary ACD/Labs format as a file which we will call EXAMPLE1.SK2.

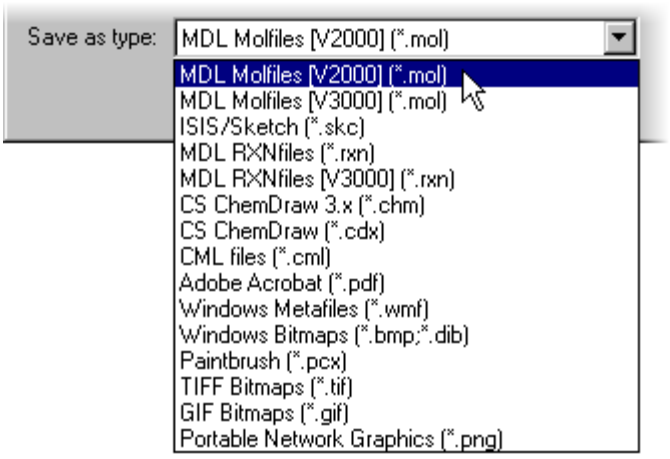
1. From the **File** menu, choose **Save**.
2. In the **Save Document As** dialog box that appears, specify the name and location of the file to which the work should be placed, and click **Save**.

> **Note** If you want to change the name or location of an existing .SK2 file, from the **File** menu, choose **Save As**.
>
> To save all of the open documents at once, from the **File** menu, choose **Save All**.

2.6.2 Saving Structure to 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 molecular structures.

1. Select the structure you want to save.
2. From the **File** menu, choose **Export** to display the corresponding dialog box.
3. Specify the name and location of a molfile to be created.
4. In the **Save as type** box, select ***MDL Molfiles [V2000] (*.mol)***:



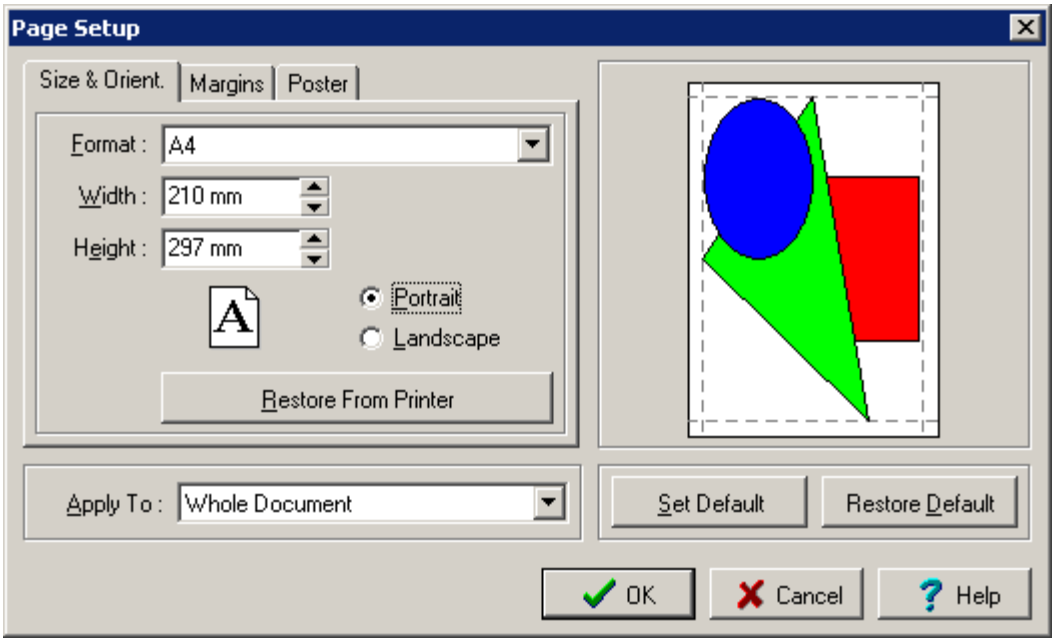
5. Click **Save**.

2.6.3 Printing ACD/ChemSketch Document

Another way to preserve your work is to print a report.

Before start printing, verify the page setup settings:

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



2. Click **OK** to save settings.

Now, you are ready to print your work:

1. On the General toolbar, click **Full Page**  to see how the page will look on a printout.
2. If necessary, move the objects on the page to arrange them properly.
3. From the **File** menu, choose **Print** or, on the General toolbar, click  to display the **Print** dialog box where you can specify the page range and the number of copies to be printed.
4. Click **Print**  .
5. Keep the EXAMPLE1.SK2 file open.

2.6.4 Embedding ACD/ChemSketch Structure into Third-Party Document

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

1. Select the required structure(s) in the ACD/ChemSketch page.
2. Copy the selection to the Clipboard using one of the following ways:
   - On the General toolbar, click **Copy**  ;
   - 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 the Clipboard contents using the **Paste** command of that application.

> **Important** When pasting structures copied from ACD/ChemSketch to third-party 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 Object** or **Picture (Windows Metafile)** option. The former inserts the structure as an OLE object thus allowing you to edit the inserted structure via ACD/ChemSketch later by double-clicking the picture.

3. Drawing More Complex Structures

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 an atom's charge;
- Draw cations and anions;
- Specify type of bonds (double, triple, coordination, Markush, *etc.*);
- Generate stereo descriptors; and
- Change various atomic properties.

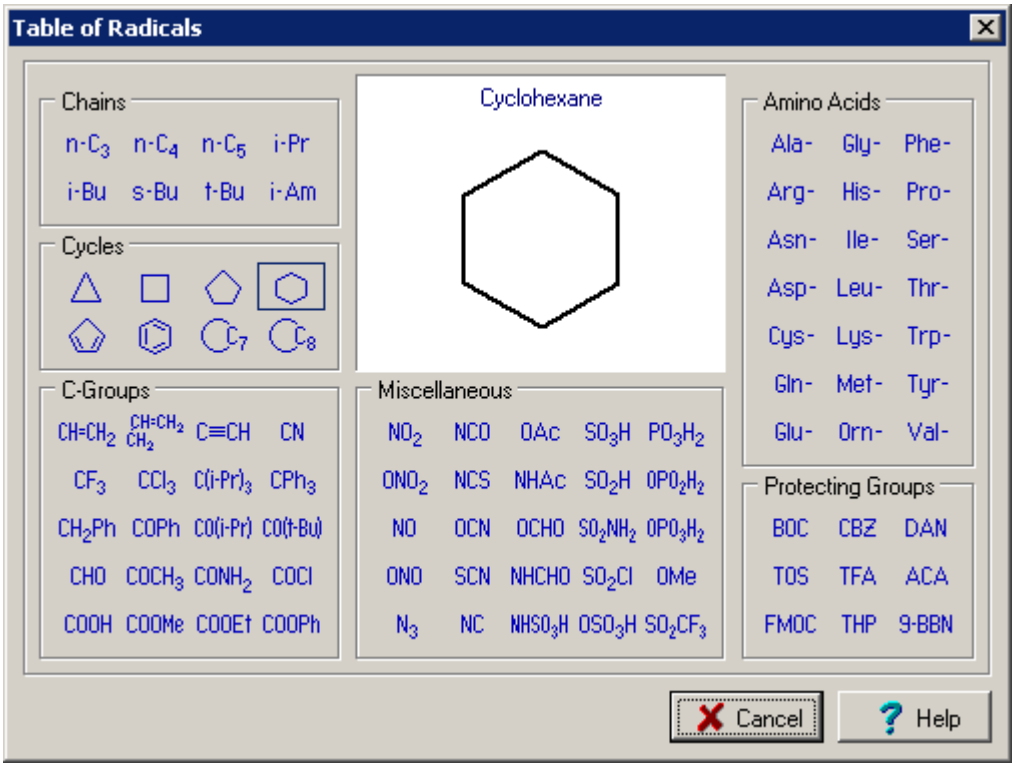
3.2 Using the Table of Radicals

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

1. With the EXAMPLE1.SK2 file still open in the workspace, on the General toolbar, click **New Page**  to start new drawing in a new page (Page 3) of the same document.
2. To illustrate the work with the Table of Radicals, clear the References toolbar: double-click blank space of the References toolbar, and then, in the message box that appears, click **Yes**. The radical buttons will be removed from the toolbar.

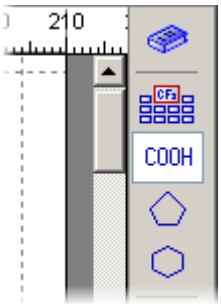
> **Tip** To turn the References toolbar to the default view, right-click the toolbar, and then, in the shortcut menu that appears, select **Reset Toolbar**.

3. On the References toolbar, click **Table of Radicals**  to display the corresponding panel:



4. Under **Cycles**, click **Cyclohexane**  to place and select a **Cyclohexane** button on the References toolbar on the right side of the screen while closing the panel. Note that the template's outline is attached to the mouse pointer.

5. Repeat Steps 3-4 for **Cyclopentane**  and **Carboxyl**  to place their buttons on the References toolbar as well:

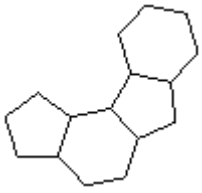


3.3 Using Ring Structures

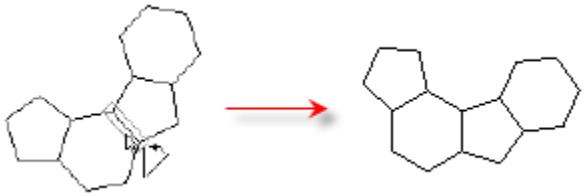
Now, we shall draw a structure of *hexadecahydrocyclopenta[c]fluorene-3,4,5,7,8,9-hexacarboxylic acid*:

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**  .
4. Now point to the bond as shown below, and then click to create the following *octahydro-1H-indene* structure:

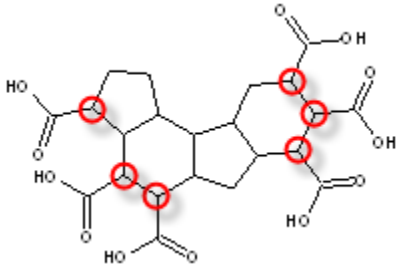
5. Repeat these steps to create the following structure:



6. On the Structure toolbar, click **Set Bond Vertically**  then click the bond as shown below to rotate the structure around this bond to obtain the following:



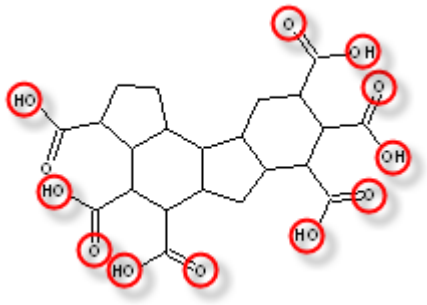
7. On the References toolbar, click **Carboxyl**  .
8. Click the indicated atoms to sprout carboxyl groups from them to obtain the following acid:



> **Note** The CHAPTER3.SK2 file (Page 1/7) with this structure can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

3.4 Deleting Atoms and Groups

In the drawn structure, we are going to delete the indicated atoms (*i.e.*, oxo- and hydroxyl groups):



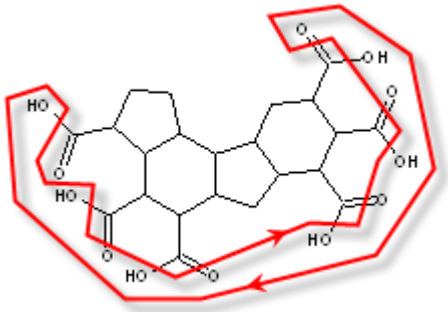
You can do this in two ways:

- By deleting each atom one by one (as covered in Section 2.2.4); or
- By deleting several atoms simultaneously (as described in the following section).

3.4.1 Deleting Several Atoms Simultaneously

With the help of the Lasso tool (introduced in Section 2.2.12), you can delete all of the required structural elements at once:

1. On the Structure toolbar, ensure that the **Lasso** selection mode  in on. Note that the **Select/Move**  tool becomes active.
2. Drag to include all of the specified atoms in the closed Lasso line to select them:

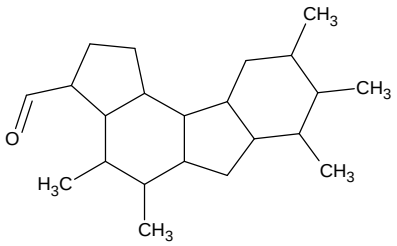


> **Note** The red line on this picture shows the suggested path of enclosing the desired groups into selection, and it will not appear as such in your workspace. Only the atoms within the lassoed space will be selected individually.

3. In case of inaccurate selection, click anywhere in the empty space of the page to deselect all of the atoms, and then try to select them again.

> **Tip** You can also select the atoms one by one or by several groups while holding down SHIFT.

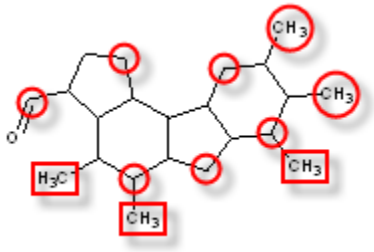
4. Delete all of the selected atoms of the structure by pressing DELETE:



> **Note** The CHAPTER3.SK2 file (Page 1/7) with this structure can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

3.5 Replacing Atoms and Groups

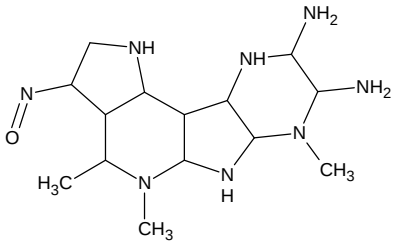
Now, let's replace the indicated carbon atoms and methyl groups with atoms of nitrogen and oxygen:



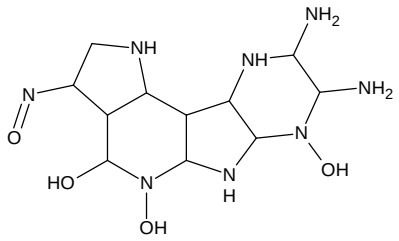
1. Ensure that the **Draw Normal** drawing tool is selected on the Structure toolbar.

> **Note** You cannot replace atoms with the **Draw Continuous** tool (for more details on this tool, refer to Section 2.2.8).

2. On the Atoms toolbar, click **Nitrogen** N, and then click all of the atoms and groups indicated with arrowed cycles on the above structure:



3. On the Atoms toolbar, click **Oxygen** O, and then click the three methyl groups indicated with red rectangles.



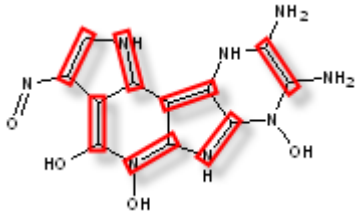
> **Note** The CHAPTER3.SK2 file (Page 1/7) with this structure can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

3.6 Setting Double Bonds

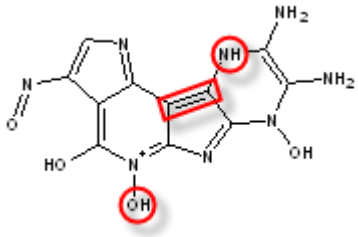
Finally, we shall draw double bonds in the structure:

1. With any of the **Draw Normal**, **Draw Continuous**, or **Draw Chains** tools active, click single bonds indicated below to turn them to double bonds:

> **Tip** Example of triple bonds drawing is given in Section 2.2.2.



2. Using the **Change Position** button, the structure's appearance can be "fine-tuned". Click this button on the Structure toolbar, 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:

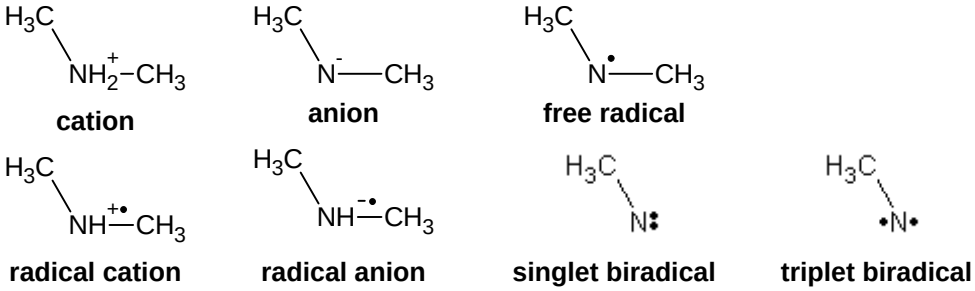


> **Note** The CHAPTER3.SK2 file (Page 1/7) with this structure can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

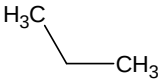
3. On the General toolbar, click **Save File**, then click **New Page**.

3.7 Setting Charges and Defining Anions and Cations

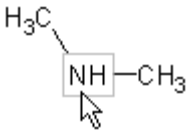
In the new ACD/ChemSketch page (Page 4), we will draw the following set of structures:



1. On the Atoms toolbar, click **Carbon** C (making sure that the **Draw Normal** tool becomes active), and then click three times at the same point of the workspace to draw the following *propane* structure:

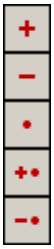


2. On the Atoms toolbar, click **Nitrogen** N, and then click the middle carbon atom to replace it with the nitrogen one:



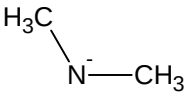
3. Select the created *N-methylmethanamine* structure, press CTRL+C to copy it to the Clipboard, and the paste five more duplicates of the structure below the first one by pressing CTRL+V repeatedly.

4. On the Atoms toolbar, click the lower right triangle of the **Increment (+) Charge** + to expand the Charges/Radicals menu containing the following buttons:

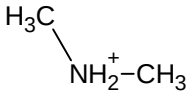


Increment (+) Charge
Decrement (–) Charge
Radical
Positive Radical Ion
Negative Radical Ion

5. From the Charges/Radicals menu, choose **Decrement (–) Charge** – tool (note that the mouse pointer is changed to –), and then click the NH group of the topmost structure to make it a *dimethylazanide* anion:

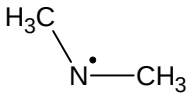


6. Right-click within the workspace to quickly switch mode of to the mouse pointer to (or choose the corresponding **Increment (+) Charge** tool from the Charges/Radicals menu), and click the NH group of the second structure to make it an *N-methylmethanaminium* cation:

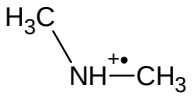


> **Note** When you change the charge of a ***nonmetal*** atom using the **Increment (+) Charge** or **Decrement (–) Charge** tools, the corresponding number of hydrogen atoms is automatically added to it, or removed from it, to preserve proper chemical valence. If you change the charge of a ***metal*** atom, 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 in the **Periodic Table of the Elements** dialog box (for more information, refer to Section 2.2.7).

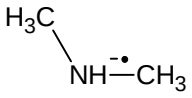
7. From the Charges/Radicals menu, choose **Radical** (the mouse pointer is changed accordingly to), and click the NH_2 group of the third structure to draw a free *dimethylamin* radical:



8. Right-click in the workspace to quickly switch mode of to the mouse pointer to (or choose the corresponding **Positive Radical Ion** tool from the Charges/Radicals menu), and click the NH group of the fourth structure to draw the *dimethylamin* radical cation:

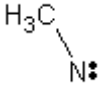


9. Right-click in the workspace to quickly switch mode of to the mouse pointer to (or choose the corresponding **Negative Radical Ion** tool from the Charges/Radicals menu), and click the NH group of the fifth structure to draw the *dimethylamin* radical anion:

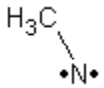


10. On the General toolbar, click **Delete**, and then click one methyl group in the last structure to turn it to *methanamine*.

11. From the Charges/Radicals menu, choose **Radical**, and click the NH group of the *methanamine* structure two times until the following singlet *methylimin* biradical is obtained:



12. Click the structure again with the radical tool to obtain the triplet *methylimin* biradical:



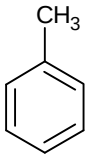
> **Note** The CHAPTER3.SK2 file (Page 2/7) with these seven structures can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

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

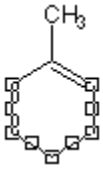
3.8 Drawing Markush Bonds

To denote structures with an undefined attachment point, you can use one of the Markush Bond tools provided by ACD/ChemSketch:

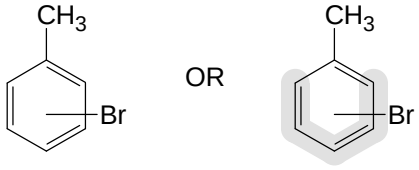
1. On the References toolbar, click **Table of Radicals** to display the corresponding panel.
2. On the panel, click **Benzene**, and then click in the workspace to paste the *benzene* structure.
3. On the Atoms toolbar, click **Carbon** (note that the **Draw Normal** tool is automatically enabled).
4. Click the topmost atom of benzene structure to sprout up a methyl group creating *toluene*:



5. On the Atoms toolbar, click **Bromine**.
6. Using the **Select/Move** tool, select five lower atoms of the structure:



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



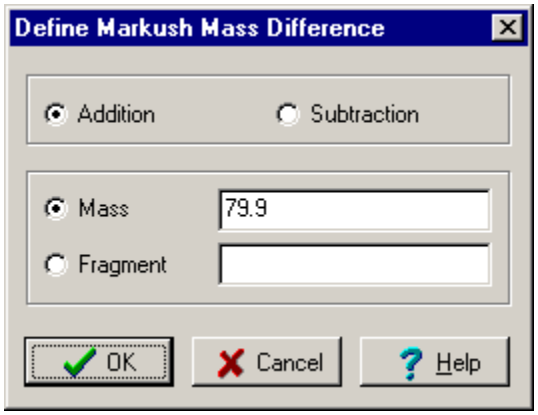
On this structure, the Br atom might be connected to any of the five carbon atoms of toluene.

> **Note** The CHAPTER3.SK2 file (Page 3/7) with these structures can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

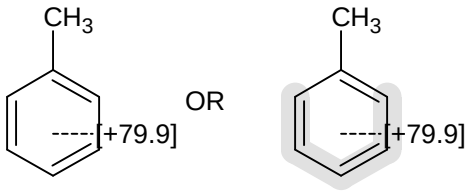
3.8.1 Markush Bond with Added or Removed Fragment

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. Draw *toluene* structure and select non-substituted carbon aromatic atoms of the structure as described in the previous section.
2. On the Structure toolbar, click **Markush Bond with Added or Removed Fragment** button: either **Added or Removed Fragment** or **Added or Removed Fragment with Shadow**.
3. In the **Define Markush Mass Difference** dialog box that appears, select both the **Addition** and **Mass** options, and then, in the adjacent box, type *79.9*:



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



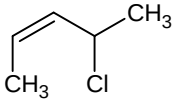
> **Note** The CHAPTER3.SK2 file (Page 3/7) with these structures can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

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

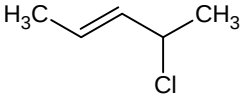
3.9 Generating Stereo Descriptors

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

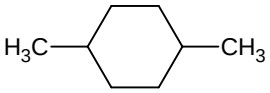
1. On the blank ACD/ChemSketch page (Page 6), draw the following set of structures using the drawing tools described above:



(2Z)-4-chloropent-2-ene

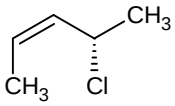


(2E)-4-chloropent-2-ene

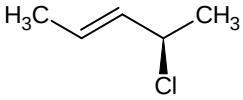


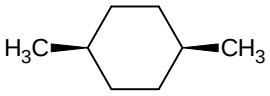
1,4-dimethylcyclohexane

2. On the Structure toolbar, click **Down Stereo Bonds**.
3. Draw the down stereo bond of the chloro substituent in the *(2Z)-4-chloropent-2-ene* structure by clicking the corresponding single C–Cl bond:



4. On the Structure toolbar, click **Up Stereo Bonds**, and repeat the previous step to draw the up stereo bonds in the other two structures as follows:



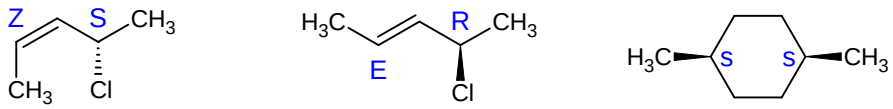


> **Tip** To draw a new stereo bond, either drag from the atom to an empty space, or simply click an existing atom (if the existing atom is of the same type as that currently active on the Atoms toolbar).
> To change the direction of a stereo bond, click this bond repeatedly.

5. Select all of the structures.

> **Note** If no structure(s) is(are) selected in the workspace, stereo descriptors 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.

6. On the **Tools** menu, point to **Generate**, and click **Stereo Descriptors** (this command available both in Structure and Draw modes). Stereo descriptors appear on the selected structures near the corresponding chiral centers and double bonds:



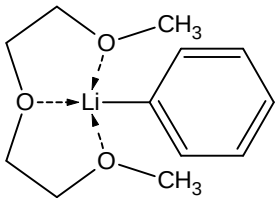
> **Note** The CHAPTER3.SK2 file (Page 4/7) with these structures can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.
>
> The following stereo descriptors are available:
>
> - S and R describe a chiral center configuration.
> - E and Z describe a double-bound configuration.
> - Small r and s describe configurations of pseudo chiral centers.
>
> To change the color of stereo descriptors:
>
> 1. From the **Options** menu, choose **Preferences** to display the **Preferences** dialog box.
> 2. Switch to the **Structure** tab, and then select the appropriate color in the **Auto/Manual Numbering Color** box. The next time you generate stereo descriptors, the new color will be used.

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

3.10 Drawing Coordination Bonds

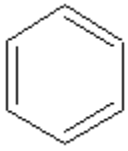
There are numerous ways to draw coordinating bonds. ACD/ChemSketch allows you to draw four different types.

We are going to draw the following structure:

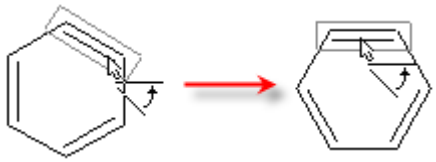


{1-(methoxy-κO)-2-[2-(methoxy-κO)ethoxy-κO]ethane}(phenyl)lithium

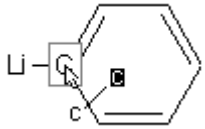
1. On the References toolbar, click **Benzene**  , and paste the benzene ring to the workspace:



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



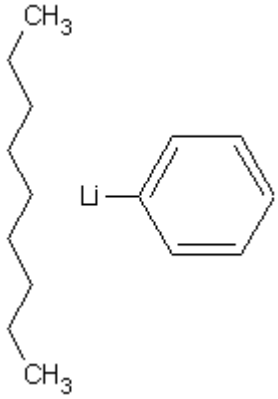
3. On the Structure toolbar, click the **Draw Continuous** tool.
4. On the Atoms toolbar, click **Periodic Table** to display the **Periodic Table of Elements** dialog box.
5. Click **Lithium** Li to select it, and then click **OK** while adding the corresponding button on the toolbar.
6. Double-click the leftmost carbon atom in the ring to sprout the Li substituent:



7. On the Structure toolbar, click **Draw Chains**, and then, on the Atoms toolbar, click **Carbon** C.
8. Holding down SHIFT, drag vertically down so that the chain being generated contains 9 elements.

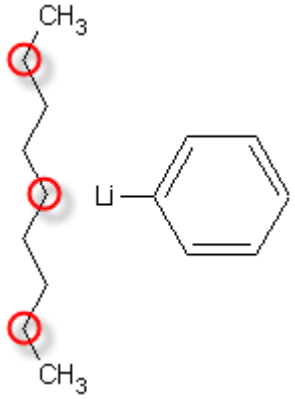
> **Tip** If the **Informative Cursor** option is selected in the **Preferences** dialog box (**General** tab), you will see the number of elements hang near the cursor when you draw the chain.

9. After dragging, select the chain, and move to the left of the drawn structure not touching it:

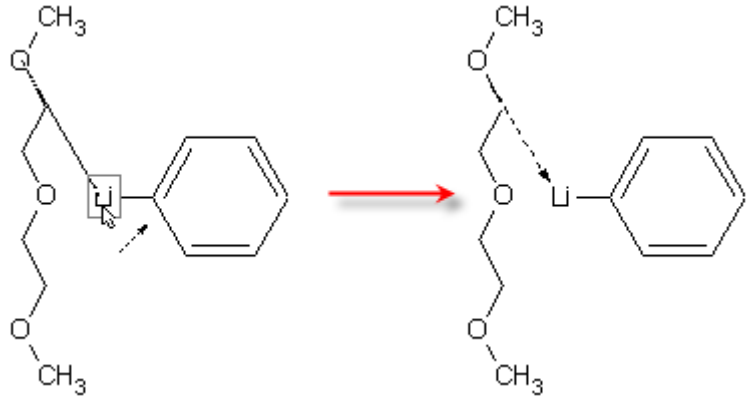


10. Switch to the **Draw Normal** tool, and, on the Atoms toolbar, click **Oxygen** O.

11. Click the buttons indicated in the picture below to replace them with the oxygen atoms:

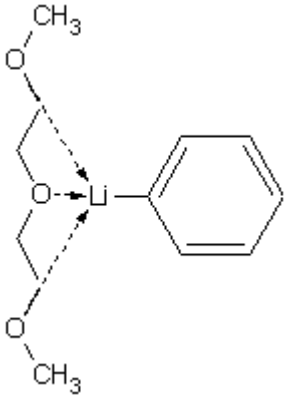


6. On the Structure toolbar, click the white triangle of the **Coordinating Bonds** tool, and choose the **Coordinating (Dashed Arrow) Bonds** tool from the menu.
7. Drag from one of the oxygen atoms to the Li atom to connect them with the coordinating bond. As you release the mouse button, the bond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

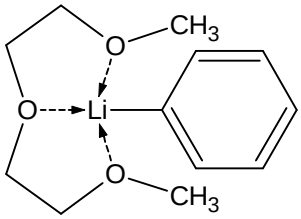


> **Note** If the bond arrow is directed the wrong way, point to the bond so that it is highlighted, and click to change the direction.

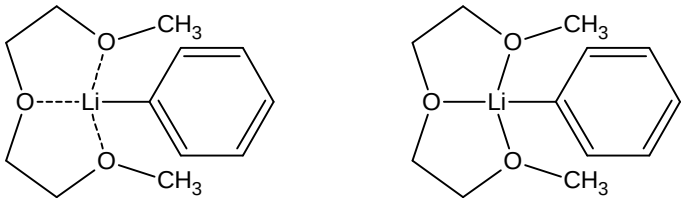
8. In the same manner, drag from other oxygen atoms to Li to draw other bonds:



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



To practice different Coordinating Bonds tools (**Coordinating (Dashed) Bonds** and **Coordinating (Solid) Bonds**), you can also try drawing the following coordination bonds:



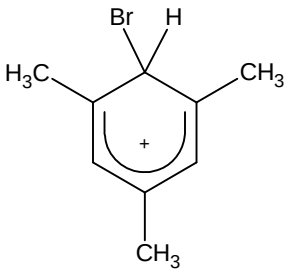
> **Note** Even looking as common bonds, coordinating bonds do not affect valences and charges of connected atoms. All the types are coded in the same way, so all the three drawings above describe the same structure.
>
> The CHAPTER3.SK2 file (Page 5/7) with these three structures can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

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

3.11 Delocalized Charges and Curves

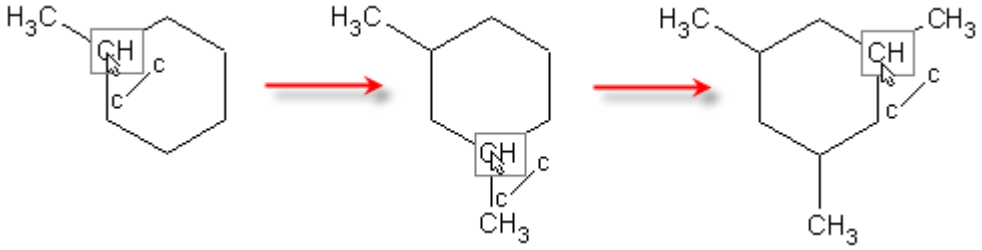
The delocalized bonds and charges can be used to draw reaction intermediates, delocalized charges and organometallic structures with multicentral coordination.

To practice this type of bonds, we are going to draw the following structure:

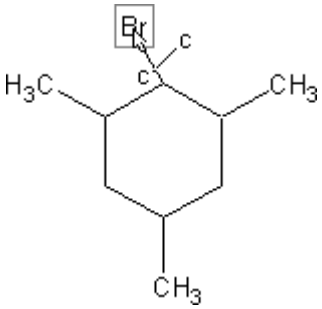


1. On the References toolbar, click **Cyclohexane**, and paste *cyclohexane* structure into the workplace.
2. On the Atoms toolbar, click **Carbon**.

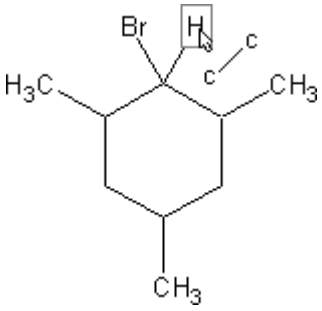
3. By clicking the carbon atoms in *meta* positions of the ring, sprout the CH_3 groups:



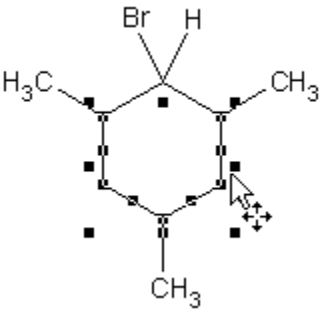
4. On the Atoms toolbar, click **Bromine** Br, and drag from the upper carbon atom of the ring to sprout a new bond:



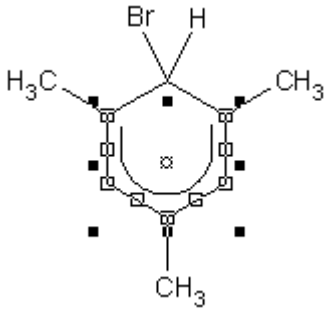
5. Click **Hydrogen** H, and drag from the same atom to sprout one more bond:



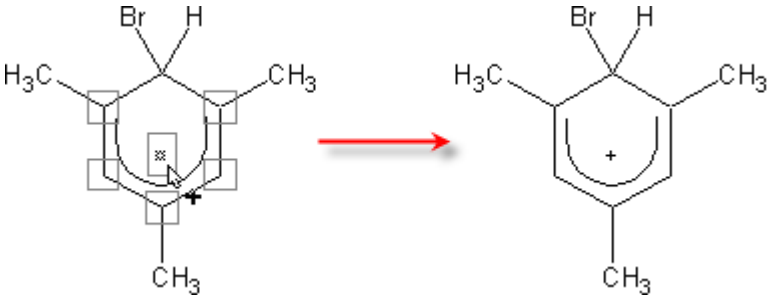
6. Click the **Select/Move** button.
7. Hold down SHIFT and click one by one the bonds so that they become selected, as shown on the picture below:



8. On the Structure toolbar, click the **Solid Delocalization Curve** tool (it is selected by default from the Delocalization Curve tools menu) to apply it to the selected bonds:



9. On the Atoms toolbar, click **Increment (+)Charge** +, then 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.

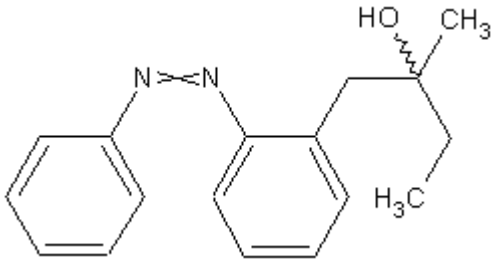
10. Now, try to draw the following structure yourself using another Delocalization Curve tool (**Dotted Delocalization Bond**) to practice the delocalized bond drawing:

> **Note** The CHAPTER3.SK2 file (Page 6/7) with these two structures can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

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

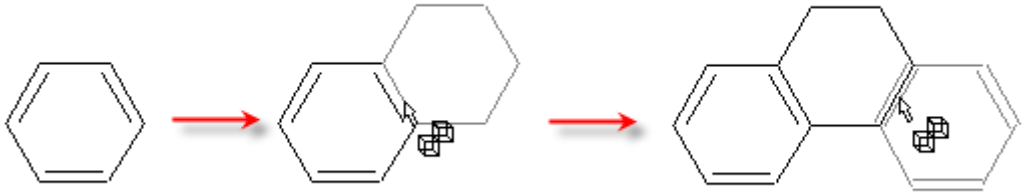
3.12 More Bond Types

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



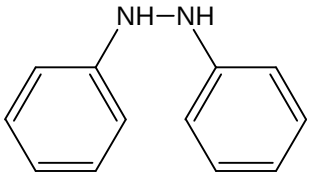
2-methyl-1-[2-(phenyldiazenyl)phenyl]butan-2-ol

1. Alternately applying the **Benzene** and **Cyclohexane** tools from the References toolbar, draw the following structure as shown below:

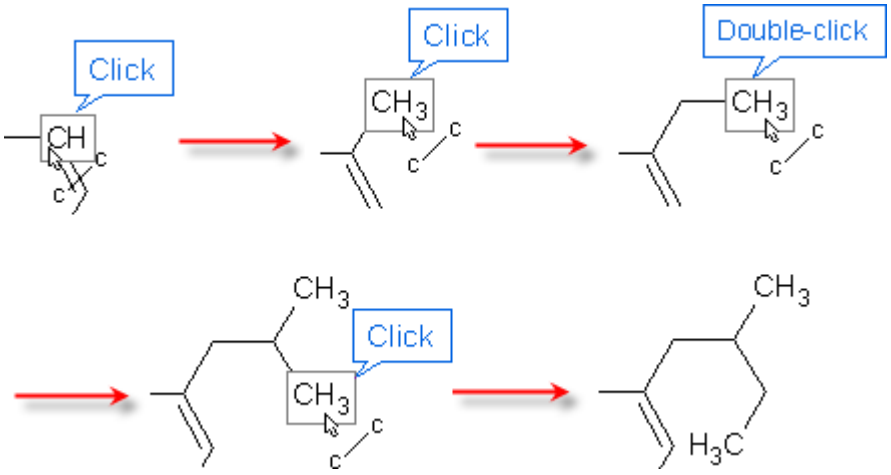


> **Tip** On the Structure toolbar, click **Set Bond Horizontally** to rotate the first inserted benzene template.

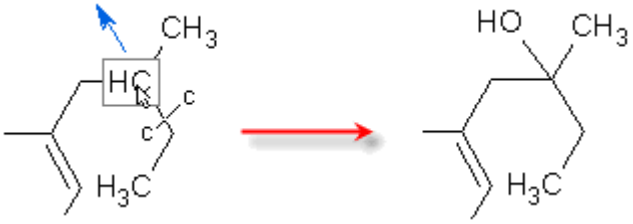
2. On the General toolbar, click **Delete**, and then click central single bond between benzene rings to remove it.
3. On the Atoms toolbar, click **Nitrogen**, and click CH_2 groups to replace them with NH ones:



4. On the Atoms toolbar, click **Carbon** C, and add *2-methylbutyl* fragment by sequentially clicking the atoms as shown below:



5. On the Atoms toolbar, click **Oxygen** O, and then drag from the indicated atom left and up to sprout an hydroxyl group:



6. On the Structure toolbar, click the white triangle of the **Undefined Stereo Bonds** button to display Special Bonds menu containing more bond types.

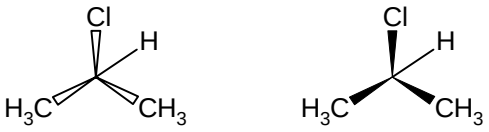
7. Click **Undefined Double Stereo Bonds** to select it, and then click the indicated single bond to replace it with the undefined type:

8. From the same Special Bonds menu of the Structure toolbar, choose **Undefined Stereo Bonds**, and click the C–OH bond to replace it with the undefined type:

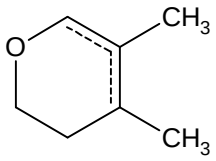
As a result, the structure shown at the beginning of this section should be created.

9. To practice the drawing of other bond types available from the Special Bonds menu, try to draw the following structures:

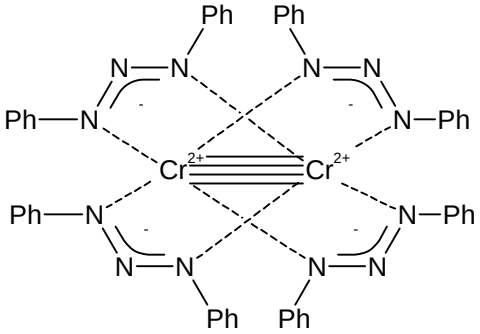
- ***Hollow wedges*** are used sometimes to describe spatial arrangement of atoms. Hollow bonds are equal to more common up stereo bonds:



- ***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:

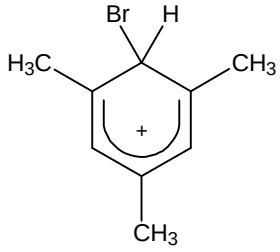


> **Note** The CHAPTER3.SK2 file (Page 7/7) with these five structures can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

3.13 Changing Atom Properties

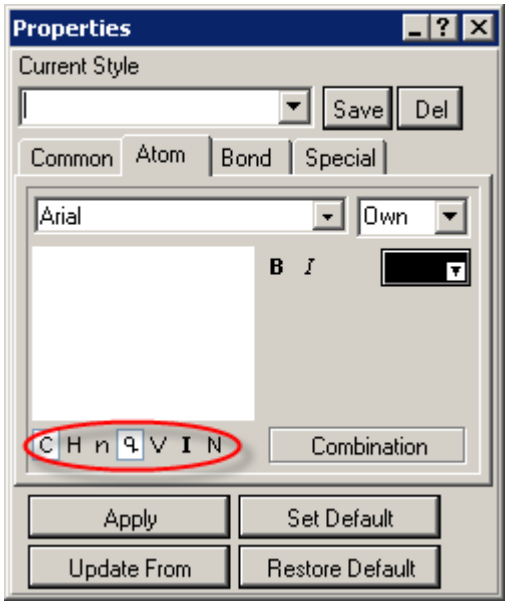
If you want to display the valence or the isotopic mass of an atom of a structure drawn in ACD/ChemSketch—or even change the typeface or the size of the atom identification—you should use the **Properties** panel.

You can use the structure drawn in Section 3.11 on the ACD/ChemSketch page 8 of the example document. We are going to change the size of the plus sign and make the visible atom symbols bold:



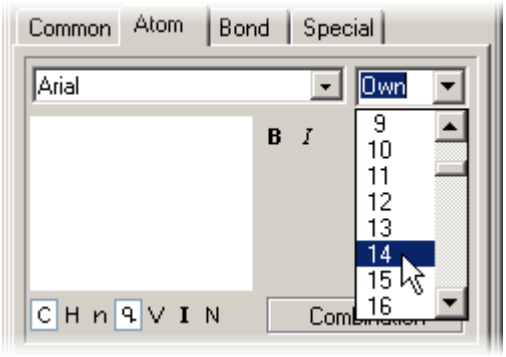
> **Note** The CHAPTER3.SK2 file (Page 6/7) with this structure can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

1. On the Structure toolbar, click **Select/Move**  .
2. Point to the plus sign in the structure, and double-click. The **Properties** panel with the **Atom** tab active appears:

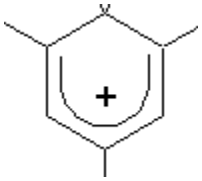


As you can see, the buttons located below the preview area allow you to specify the style settings for seven possible atom attributes: Atom Symbol (C), Hydrogen (H), Hydrogen Index (n), Charge (q), Valence (V), Isotope (I), and Numbering (N).

3. In the drop-down list adjacent to the Font, select ***14***:



4. Click **Apply** 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; after all click the rightmost button on the title bar of the panel to close it.

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

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

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 **Clean Structure**  tool for 2D-optimization;
- 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.

> **Note** Prior to performing any of the procedures described below, ensure that you are in the Structure mode of ACD/ChemSketch.

4.2 2D-Optimization

The **Clean Structure**  tool can be applied for 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 perfect structures as demonstrated in the examples below.

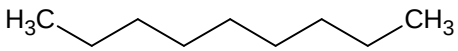
4.2.1 Creating the Structure of Cyclic Alkanes

Using the following technique, you can quickly draw cyclic alkanes.

Here's how to draw a *cyclononane* structure:

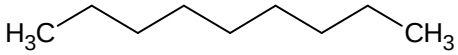
1. Being in the new blank ACD/ChemSketch document, on the Atoms toolbar, click **Carbon**  .

2. On the Structure toolbar, click **Draw Chains**, and drag in the workspace to draw a 9-member chain on *nonane*:

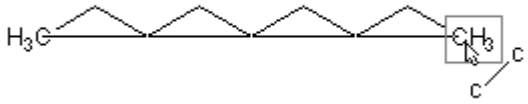


> **Tip** If the **Informative Cursor** option is selected in the **Preferences** dialog box (**General** tab), you will see the number of elements hang near the cursor when you draw the chain.

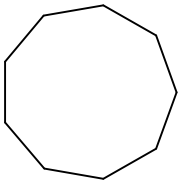
3. On the Structure toolbar, click **Flip Top to Bottom** to turn the structure upside down (this step is optional):



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



5. On the Structure toolbar, click **Clean Structure** to obtain the following cycle:



6. Try to draw C_{10}- and C_8-rings using the above technique.

> **Note** The CHAPTER4.SK2 file (Page 1/9) with these three structures can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

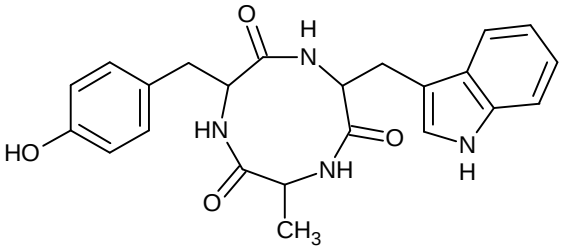
7. On the General toolbar, click **Save File**, in the **Save Document As** dialog box that appears, specify the name and location of the file to which the work should be placed, and click **Save**.

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

4.2.2 Creating the Structure of a Cyclic Peptide

This section is based on the PEPT.EXE movie which can be found in the \\MOVIES\CHEMSK folder.

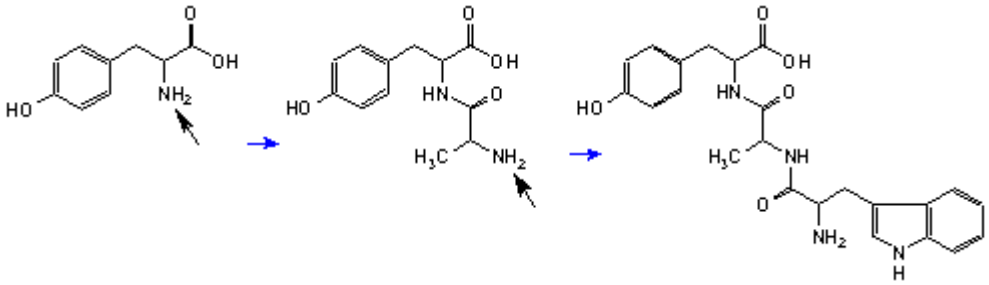
Let's draw the cyclic Tyr-Ala-Trp peptide using the **Clean Structure** tool:



1. On the General toolbar, click the **Open Template Window** button to display the **Template Window** dialog box, and switch to the **Amino Acids** tab.

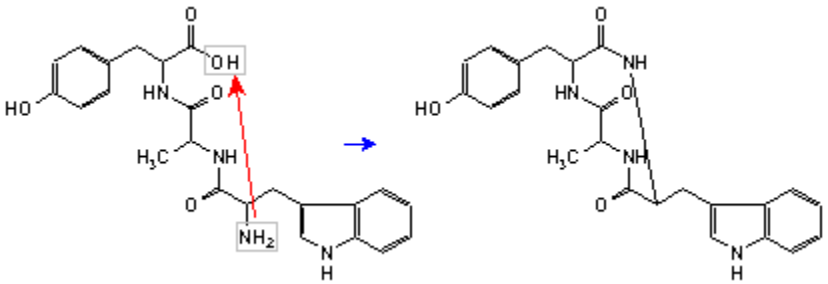
   > **Note** If the **Amino Acids** tab is absent at the left part of the dialog box, choose its name from the leftmost drop-down list at the top of the dialog box.

2. Ensure that the ***1(4) Acids*** set of amino acids is chosen in the rightmost drop-down list at the top of the dialog box.
3. Click the ***template*** of Tyrosine (not its ***name***), and then click within the workspace to paste the structure.
4. From the Table of Radicals (for more information, refer to Section 3.2), choose sequentially **Alanine** Ala- and **Tryptophan** Trp-, and attach the corresponding radicals as follows:



   > **Tip** You can flip the template's outline before placing it in the workspace by pressing TAB.

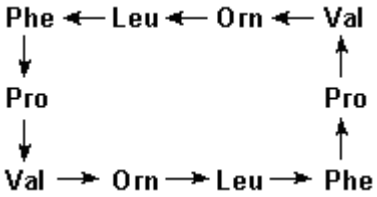
5. Right-click to quickly switch to the **Select/Move** tool, and drag the NH_2 group to the OH group as shown:



6. On the Structure toolbar, click **Clean Structure** to obtain the required structure.
7. Using selection and rotation tools from the Structure toolbar, bring the structure to the desired appearance.

> **Note** The CHAPTER4.SK2 file (Page 2/9) with this structure can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

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



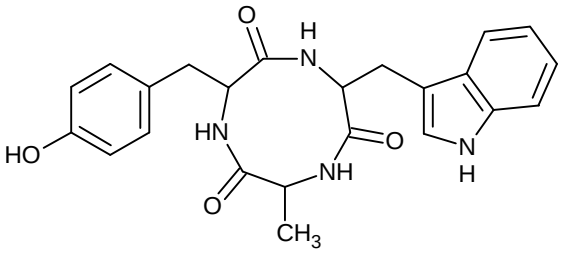
4.3 SMILES Notations

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

Let's create a SMILES string for the cyclic peptide drawn in Section 4.2.2.

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



Oc1ccc(cc1)CC4NC(=O)C(C)NC(=O)C(Cc3cnc2ccccc23)NC4=O

You can now select the text string and press CTRL+C to copy it to the Clipboard, and then paste it into any external text editor (*e.g.*, Windows Notepad) as text using the **Paste** command from the editor's menu or by pressing 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 the generation procedure. 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

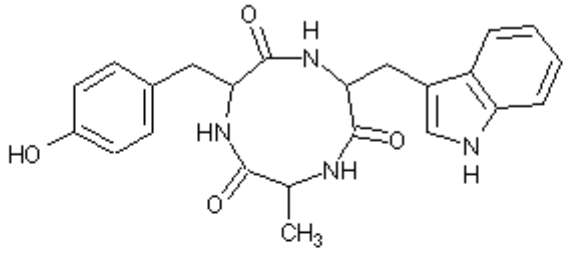
Now we will try the inverse task: generation of structures from the SMILES strings.

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:

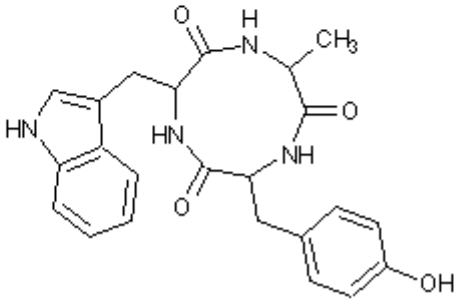
Oc1ccc(cc1)CC4NC(=O)C(C)NC(=O)C(Cc3cnc2ccccc23)NC4=O

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 that was generated in the previous section:



Source structure

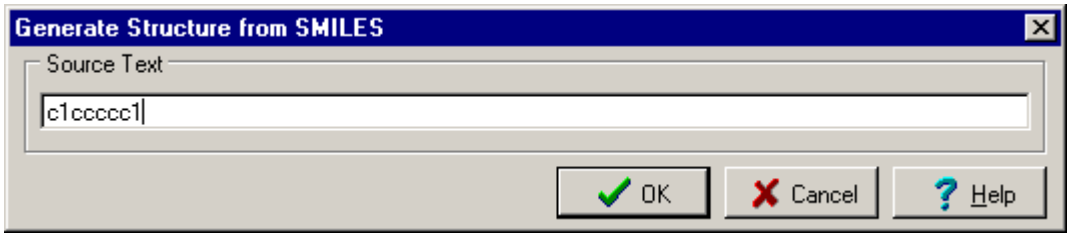
Oc1ccc(cc1)CC4NC(=O)C(C)NC(=O)C(Cc3cnc2ccccc23)NC4=O



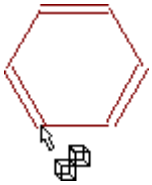
Generated structure

> **Note** The CHAPTER4.SK2 file (Page 2/9) with these structures can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

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 enter the string manually—for example the string for *benzene*:



3. Click **OK**. The generated structure is attached to the cursor as an outline:



4. Click in the workspace to place the structure.
5. 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.

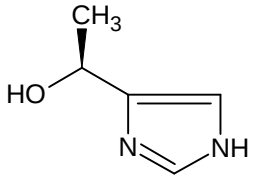
InChI procedures were developed under IUPAC project. The technical development was carried out primarily at the US National Institute of Standards and Technology (NIST). More information about InChI is available on the IUPAC Web site at:

http://www.iupac.org/inchi/

4.4.1 Generating InChI Notations

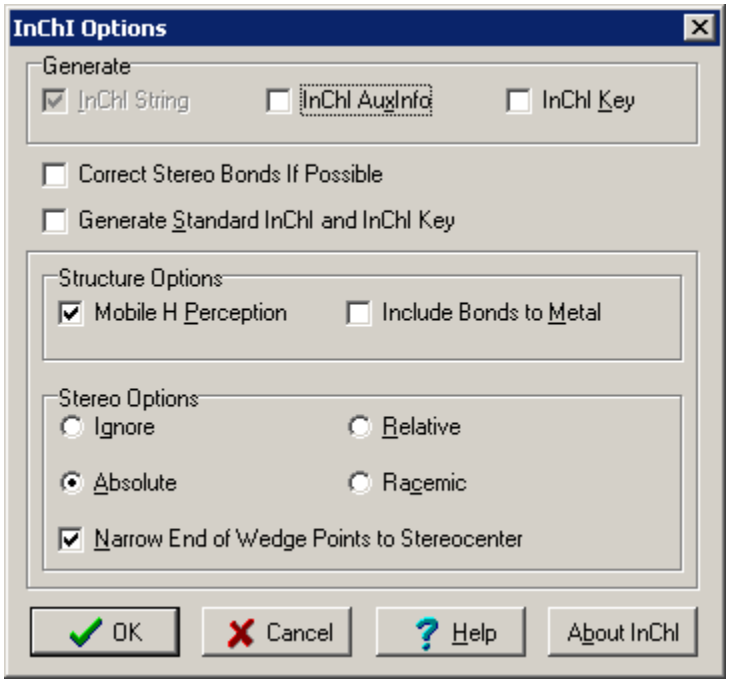
Let's create an InChI string for *(1S)-1-(1H-imidazol-4-yl)ethanol*.

1. Using the obtained skills, draw the following structure:

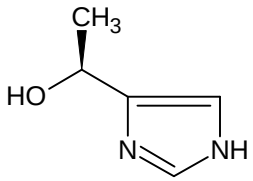


2. On the **Tools** menu, point to **Generate**, and then choose **InChI Options**.

3. In the dialog box that appears, specify the options as shown below, and click **OK**:



4. 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** The CHAPTER4.SK2 file (Page 3/9) with this structure can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

You can now select the text string and press CTRL+C to copy it to the Clipboard, and then paste it into any external text eitor (*e.g.*, Windows Notepad) as text using the **Paste** command from the editor's menu or by pressing CTRL+V.

> **Note** If you have several structures drawn on one page and you want to generate the InChI string for all of them, you do not have to select them all—just leave them all unselected, and repeat the generation procedure. The InChI notation appears for all the drawn structures as one string.

5. Repeat the generation of the InChI string for the current structure 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

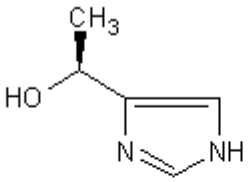
4.4.2 Generating Structures from InChI Notations

Now we will perform the inverse task: generation of a structure from an 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:

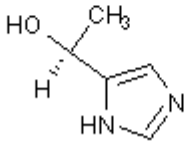
InChI=1/C5H8N2O/c1-4(8)5-2-6-3-7-5/h2-4,8H,1H3,(H,6,7)/t4-/m0/s1

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:



Source structure

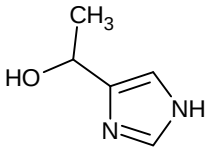
InChI=1/C5H8N2O/c1-4(8)5-2-6-3-7-5/h2-4,8H,1H3,(H,6,7)/t4-/m0/s1



Generated structure

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

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



> **Note** The CHAPTER4.SK2 file (Page 3/9) with these three structures can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

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

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.

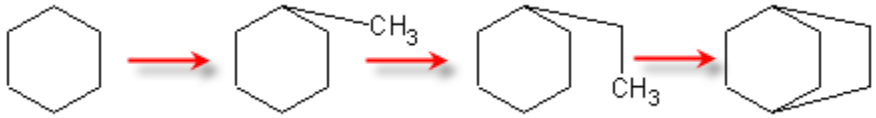
4.5.1 Creating Structure of Bicyclo[2.2.2]octane

This section is based on the BICYC.EXE movie which can be found in the \\MOVIES\CHEMSK folder.

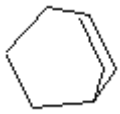
Using the following technique, you can quickly draw bicyclic alkanes.

Here's how to draw a *bicyclo[2.2.2]octane* structure:

1. From the **Options** menu, choose **Preferences**, and then, 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 References toolbar, choose **Cyclohexane**  , and 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:

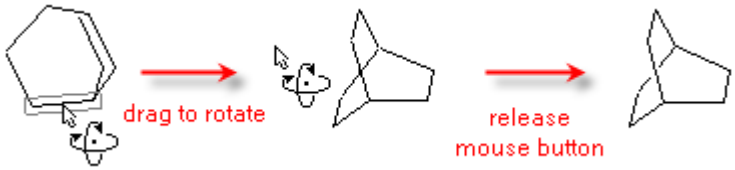


5. On the Structure toolbar, click **3D Optimization** to obtain a 3D model of the drawn structure:



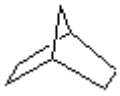
> **Note** If there is more than one structure in the workspace, you should select the structure you want to optimize in 3D using any of the selection tools: **Select/Move**, **Select/Rotate/Resize**, or **3D Rotation**.

6. If the **Switch to 3D Rotation mode** check box on 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** on the Structure toolbar.
7. Point to any atom or bond on the structure and drag over the workspace to rotate the structure until it is placed as shown:

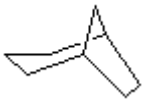


> **Note** You can choose whether the background bond will be broken or not in the structure:
>
> 1. From the **Options** menu, choose **Preferences**, and then switch to the **Structure** tab of the dialog box that appears.
> 2. In the **Bonds Intersections** area, select or clear the **Enable** check box.
>
> 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.

8. Using the above technique, draw the following bicyclic structures on your own:



Bicyclo[2.2.1]heptane



Bicyclo[3.2.1]octane

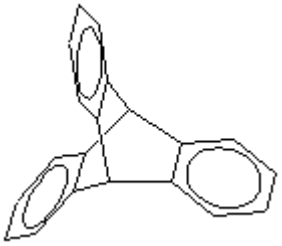
You can also choose the above structures from the corresponding templates in the **Template Window** dialog box. For more information on this dialog box, refer to Section 5.5.

> **Note** The CHAPTER4.SK2 file (Page 4/9) with these three structures can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

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

4.5.2 Creating the Structure of Triptycene

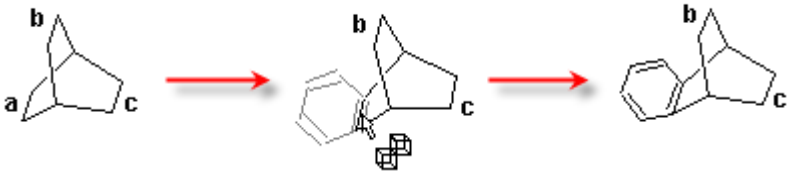
This section is based on the TRIPTYC.EXE movie which can be found in the \\MOVIES\CHEMSK folder.



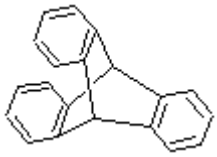
1. Draw the structure of *bicyclo[2.2.2]octane* as described in the section above.

   Tip You can also select corresponding template on the **Bicyclics** tab of the **Template Window** dialog box (for more information, refer to Section 5.5), and paste it in the workspace. If the tab is absent at the left part of the dialog box, choose its name from the leftmost drop-down list at the top of the dialog box.

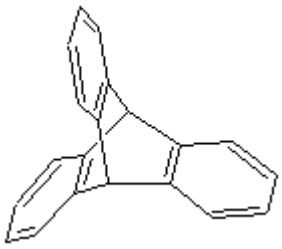
2. On the References toolbar, choose **Benzene**  .
3. Point to the bond **a**, and click to attach the benzene ring to this bond:



4. Repeat step 3 for bonds **b** and **c** to obtain the following structure of *triptycene*:



5. On the Structure toolbar, click **3D Optimization**  to obtain a 3D-model of the drawn structure:



6. If the **Switch to 3D-Rotation Mode** check box on the **Structure** tab of the **Preferences** dialog box (**Options** menu) 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**  on the Structure toolbar.
7. Point to any atom or bond of the structure and drag over the workspace to obtain the projection you want (for details, refer to the previous section).

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

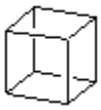
> **Note** The CHAPTER4.SK2 file (Page 5/9) with these structures can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

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

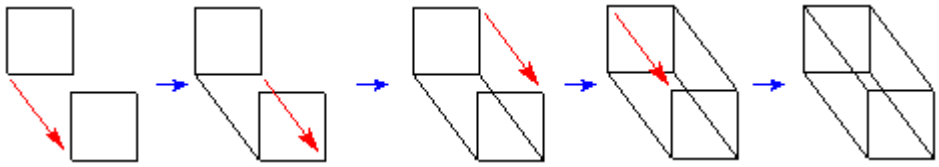
4.5.3 Creating Structure of Cubane

Using the following technique, you can quickly draw bridged polycycles.

Here's how to draw a *cubane* structure.

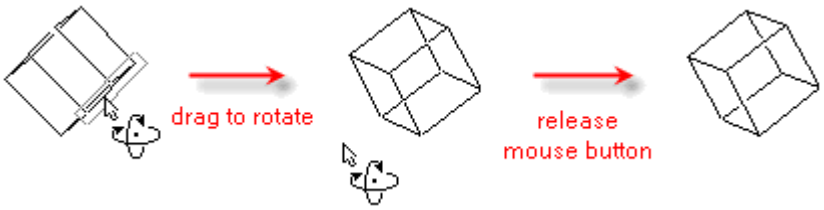


1. On the References toolbar, click **Table of Radicals**, and then choose **Cyclobutane**.
2. Click within the workspace to place 4-membered ring, and once again to place another ring below the first one.
3. On the Structure toolbar, click **Draw Normal**, and connect the corners of the cyclobutane structures with bonds by dragging from one atom to another as shown:



4. On the Structure toolbar, click **3D Optimization** to obtain the 3D model of the drawn structure.
5. On the Structure toolbar, click **3D Rotation** if it is not already selected.

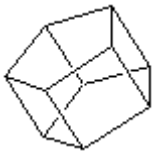
6. Point to any atom or bond on the structure, and drag over the workspace to obtain the projection you want:



> **Note** You can choose whether the background bond will be broken or not in the structure:
>
> 1. From the **Options** menu, choose **Preferences**, and then switch to the **Structure** tab of the dialog box that appears.
> 2. In the **Bonds Intersections** area, select or clear the **Enable** check box.
>
> 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.

7. Using the above technique, draw the following bridged polycycles on your own:

Prismane



Pentaprismane

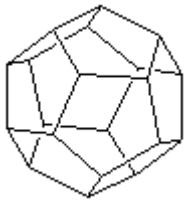
You can also choose the above structures from the corresponding templates in the **Template Window** dialog box. For more information on this dialog box, refer to Section 5.5.

> **Note** The CHAPTER4.SK2 file (Page 6/9) with these three structures can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

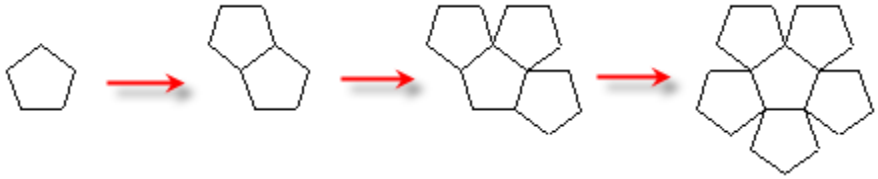
8. On the General toolbar, click **Save File**, then click **New Page**.

4.5.4 Creating the Structure of Dodecahedrane ([5]Fullerene-C_{20})

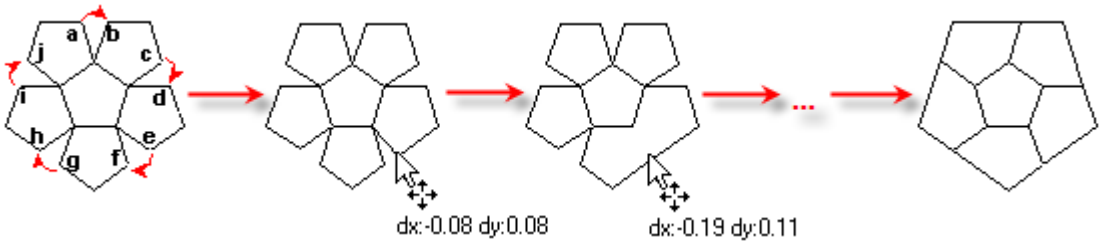
This section is based on the FULLER.EXE movie which can be found in the \\MOVIES\CHEMSK folder.



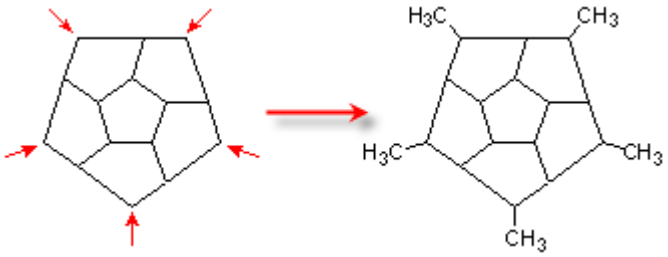
1. On the References toolbar, choose **Cyclopentane** .
2. Click in the workspace to place a cyclopentane ring.
3. Sequentially point to each bond of the ring and click to attach five other rings:



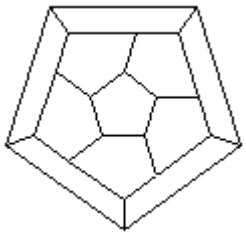
4. Right-click to quickly switch to the **Select/Move** tool.
5. Move by dragging atoms **a**, **c**, **e**, **g**, **i** to atoms **b**, **d**, **f**, **h**, **j** accordingly as shown in the following scheme to merge them:



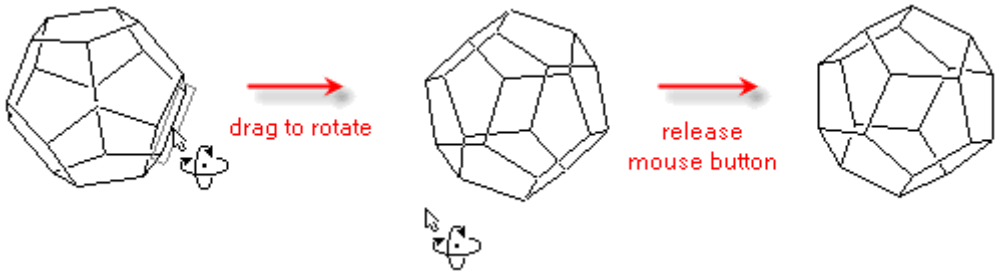
6. On the Atoms toolbar, click **Carbon** C, and then click directly carbon atoms indicated below by arrows to add five methyl groups:



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



8. On the Structure toolbar, click **3D Optimization**  to obtain the 3D model of the drawn *[5]fullerene-C_{20}-I_h* structure.
9. On the Structure toolbar, click **3D Rotation**  .
10. Point to any atom or bond on the structure, and drag over the workspace to obtain the projection you want.

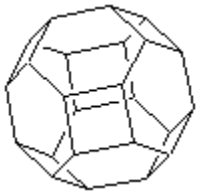


Note You can choose whether the background bond will be broken or not in the structure:

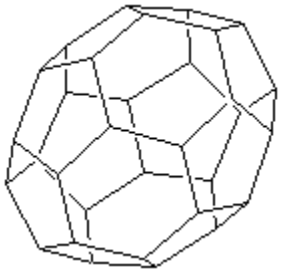
1. From the **Options** menu, choose **Preferences**, and then switch to the **Structure** tab of the dialog box that appears.
2. In the **Bonds Intersections** area, select or clear the **Enable** check box.

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.

11. Using the above technique, draw the following fullerene structures on your own:



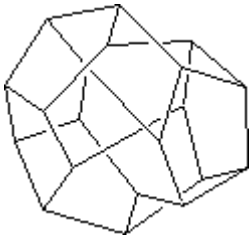
[4,6]Fullerene-C_{24}-O_h



[5,6]Fullerene-C_{32}-D_3

Tip You can also choose the above structures from the corresponding templates in the **Template Window** dialog box. For more information on this dialog box, refer to Section 5.5.

If you obtain a "Moebius" structure:



instead of a fullerene-type structure, it means than the optimization has converged to an unusual value. To fix the malfunction:

1. Click **Undo** to return to your pre-optimized structure.
2. Click **Clean Structure** or move some of the atoms slightly using the **Select/Move** tool, and then optimize the structure again.

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

Note The CHAPTER4.SK2 file (Page 7/9) with these three structures can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
To switch to the required page, use the corresponding buttons on the Status bar.

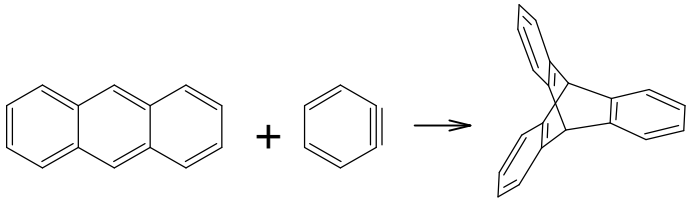
4.6 Drawing, Labeling, and Mapping Reactions

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

4.6.1 Drawing a Reaction

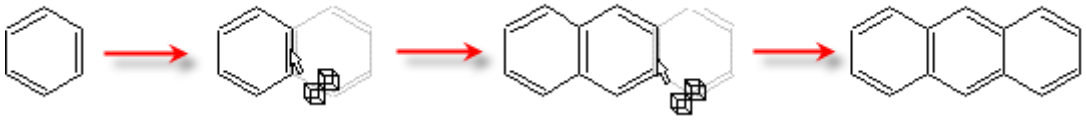
This section is based on the REACTION.EXE movie which can be found in the \\MOVIES\CHEMSK folder.

In this section, we will draw the following reaction:



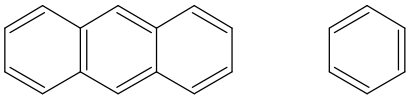
1. On the References toolbar, click **Table of Radicals**, and then choose **Benzene** (if you have recently used this template, you can find it on the toolbar).

2. Pressing TAB to flip the template's outline when necessary, draw the following structure by clicking in the workspace several times:

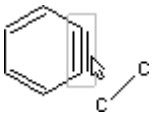


> **Note** To draw a fused-ring structure, place the cursor directly over a ring bond as shown, and then click.

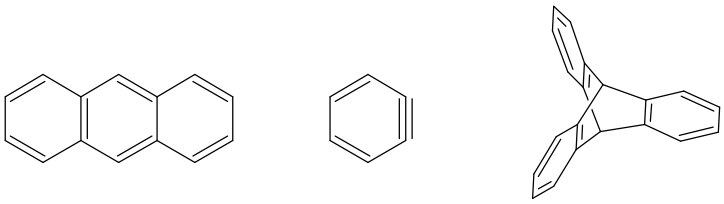
3. Press TAB to flip the outline again, and click beside the drawn structure to place a separate ring.
4. Right-click to hide the template outline:



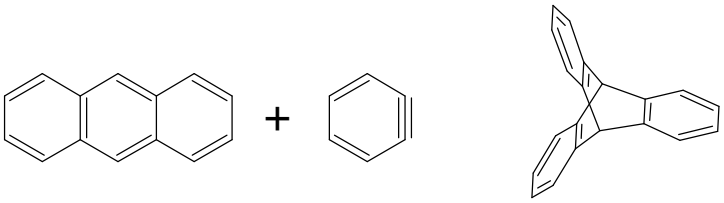
5. On the Structure toolbar, click **Draw Normal**  , and then click the bond of the *benzene* ring to make it triple:



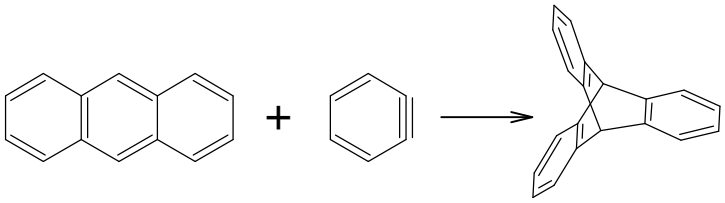
6. Draw the structure of *triptycene* as described in Section 4.5.2, and place it to the right of the other structures:



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



8. Click **Reaction Arrow**  , and then either click or drag to place the arrow as well:

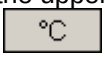


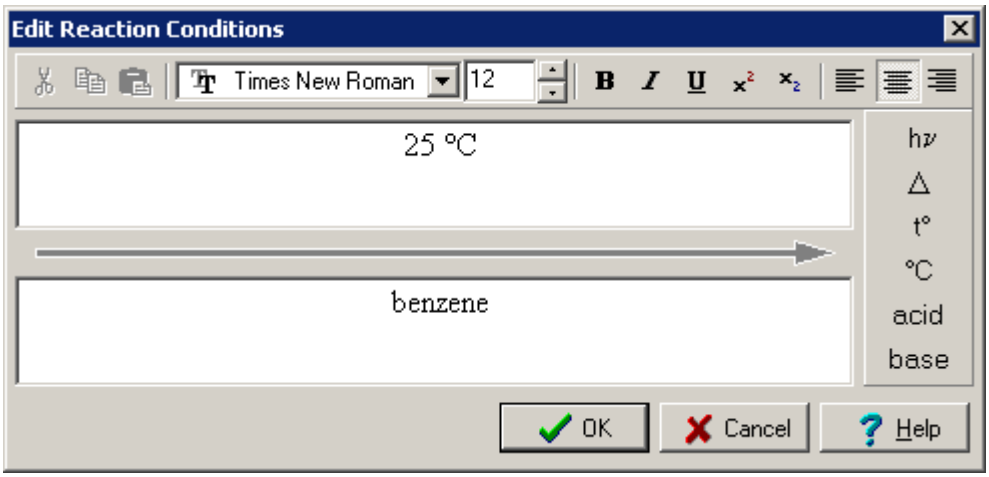
> **Note** By clicking the lower right triangle of the **Reaction Arrow**  button you can choose from a variety of reaction arrows. However, some arrows are treated as graphical objects and cannot be exported properly.

9. To move the plus sign or the arrow within the reaction as desired, click **Select/Move**  , point to the object, and then drag.

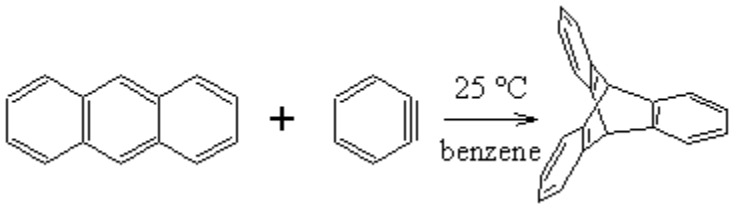
4.6.2 Labeling a Reaction

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

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 upper box of the **Edit Reaction Conditions** dialog box, type *25*, and then click **°C**  on the right toolbar of the dialog box.
4. In the lower box, type *benzene*:



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



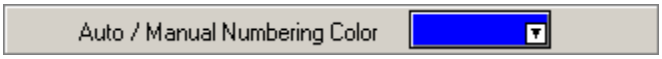
> **Note** The CHAPTER4.SK2 file (Page 8/9) with this reaction can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

4.6.3 Mapping a Reaction

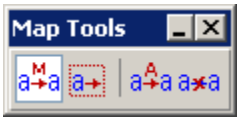
This procedure allows you to map a drawn reaction either manually or automatically. To differentiate between the automatically generated and manually inserted atom numbers, select different colors for automatic and manual mapping.

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.

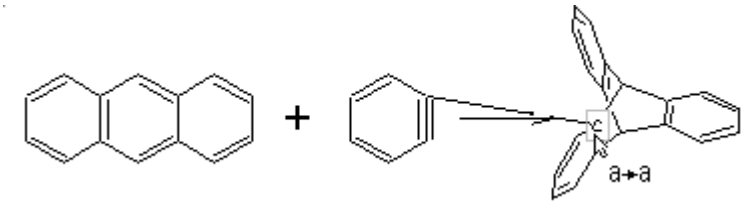


4. Click **OK**. Now, we can get down to mapping as it is.
5. On the Structure toolbar, click **Atom-Atom Map**  to display the **Map Tools** panel and enable the mapping mode:



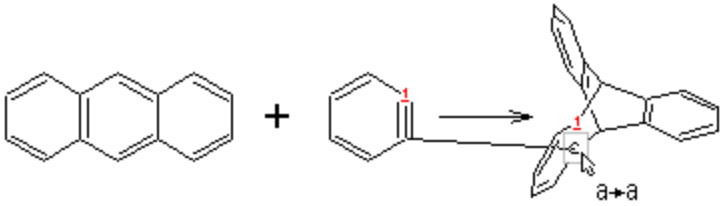
> **Note** The Manual Mapping mode is automatically enabled (the corresponding button is active).

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



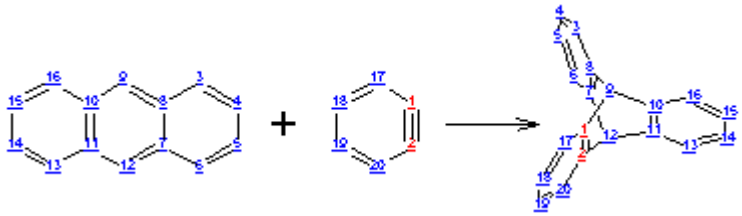
As you release the mouse button, **1** appears on the reaction near the reactant atom and near its counterpart on the product denoting manually mapped atoms.

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



As you release the mouse button, **2** appears on the reaction near the reactant atom and near its counterpart on the product denoting manually mapped atoms.

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

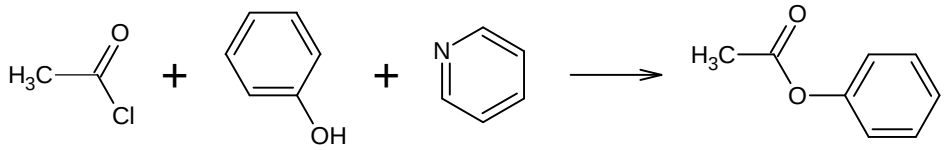


> **Note** The mapped atoms are only visible when the **Map Tools** panel is displayed.

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

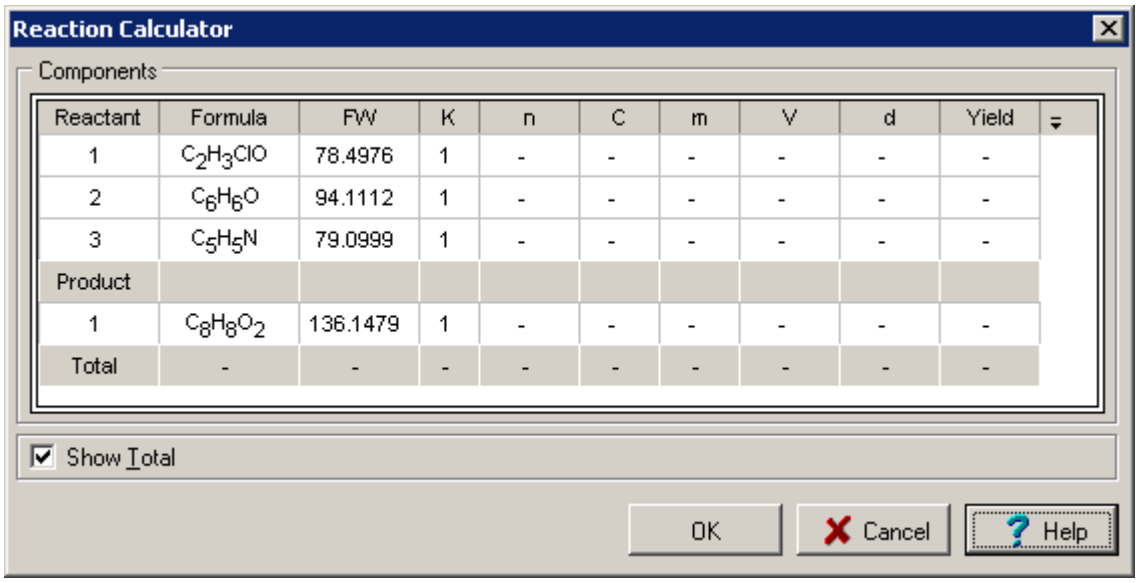
4.6.4 Calculating Reaction Data

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



acetyl chloride *phenol* *pyridine* *phenyl acetate*

1. On the Structure toolbar, click **Reaction Calculator**  , and then click the reaction arrow.
2. In the **Reaction Calculator** dialog box that appears, select the **Show Total** check box:



3. In the row that corresponds to *acetyl chloride* (C_2H_3ClO), double-click the Quantity cell (**n**) to select it, type *0.11* (in *mol*), and then press ENTER.
4. 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* (in *g/mL*). After you press ENTER, the calculated value in *mL* appears in the adjacent Volume cell (**V**).

5. Similarly, insert the following values into the corresponding cells of the Components table: for *phenol* (C_6H_6O)—*0.1* mol for quantity (**n**), for *pyridine* (C_5H_5N)—*0.11* mol for quantity (**n**) and *0.983* g/mL for density (**d**). Note that all of the dependent data is calculated automatically.
6. Double-click the Mass cell (**m**) corresponding to the *phenyl acetate*, ($C_8H_8O_2$) and type *12.9* (in *g*).
7. Press ENTER. You will see that the yield is calculated and the ***Based on*** notation appears under **Yield** in the row corresponding to phenol:

Reactant	Formula	FW	K	n	C	m	V	d	Yield
1	C_2H_3ClO	78.4976	1	0.11 mol	-	8.6347 g	7.8498 mL	1.1 g/mL	-
2	C_6H_6O	94.1112	1	0.1 mol	-	9.4111 g	-	-	Based on
3	C_5H_5N	79.0999	1	0.11 mol	-	8.701 g	8.8515 mL	0.983 g/mL	-
Product									
1	$C_8H_8O_2$	136.147	1	0.0948 mol	-	12.9 g	-	-	94.75 %
Total	-	-	-	0.32 mol	-	26.747 g	16.701 mL	-	-

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

Reactant	Formula	FW	K	n	C	m	V	d	Yield
1	C_2H_3ClO	78.4976	1	0.11 mol	-	8.6347 g	7.8498 mL	1.1 g/mL	-
2	C_6H_6O	94.1112	1	0.1 mol	-	9.4111 g	-	-	Based on
3	C_5H_5N	79.0999	1	0.11 mol	-	8.701 g	8.8515 mL	0.983 g/mL	-
Product									
1	$C_8H_8O_2$	136.1479	1	0.0948 mol	-	12.9 g	-	-	94.75 %
Total	-	-	-	0.32 mol	-	26.747 g	16.701 mL	-	-

> **Note** The CHAPTER4.SK2 file (Page 9/9) with the reaction and Components table can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

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

5. Advanced Drawing: Templates

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** dialog box for drawing DNA structures and complex biomolecular structures; and
- How to create your own templates.

> **Note** Prior to performing any of the procedures described below, ensure that you are in the Structure mode of ACD/ChemSketch.

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 of the Table of Radicals tool is fixed (invariable), the Template Window and Instant Template ones allow you to specify any atom or bond to be the binding point 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's outline 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's outline before fixing it by sequential pressing TAB.

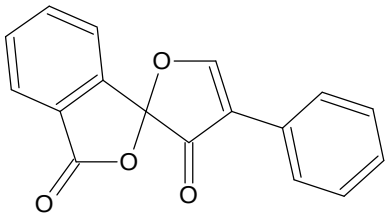
5.3 Table of Radicals

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 Structure of Fluorescamine

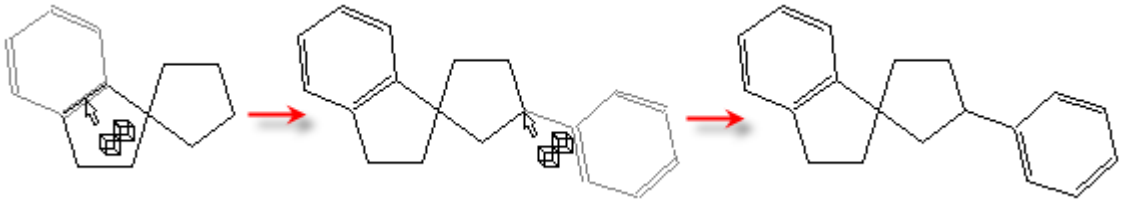
This section is based on the FLUOR.EXE movie which can be found in the \\MOVIES\CHEMSK folder.

We will draw the following structure of *4'-phenyl-3H,3'H-spiro[2-benzofuran-1,2'-furan]-3,3'-dione* using templates taken from the Table of Radicals:

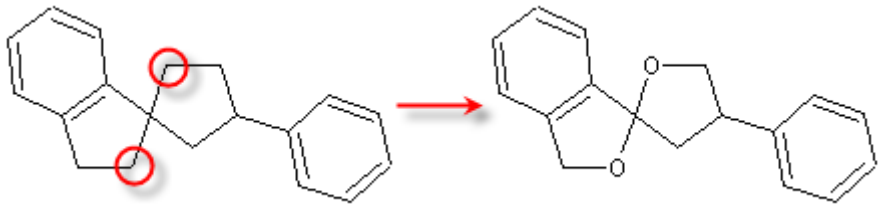


1. Being in the new blank ACD/ChemSketch document, on the References toolbar, click **Table of Radicals**  , and choose **Cyclopentane**  (if you have recently used this template, you can find it on the toolbar).
2. Click within the ChemSketch workspace to paste the *cyclopentane* ring.
3. Click the carbon atom of the ring while holding down SHIFT to obtain the spiro-connection with the second cyclopentane ring:

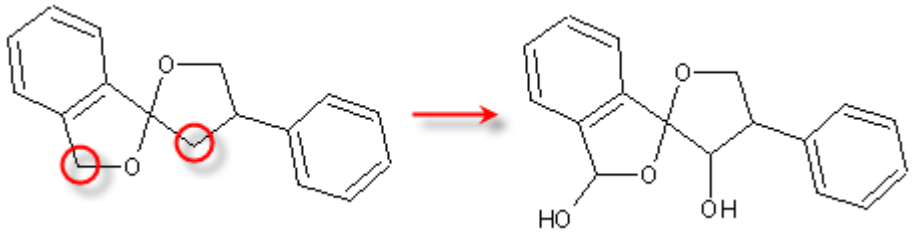
4. On the References toolbar, click **Table of Radicals**  , and choose **Benzene**  (if you have recently used this template, you can find it on the toolbar).
5. First click the indicated bond to fuse the benzene ring, and then click the indicated atom to connect the phenyl radical:



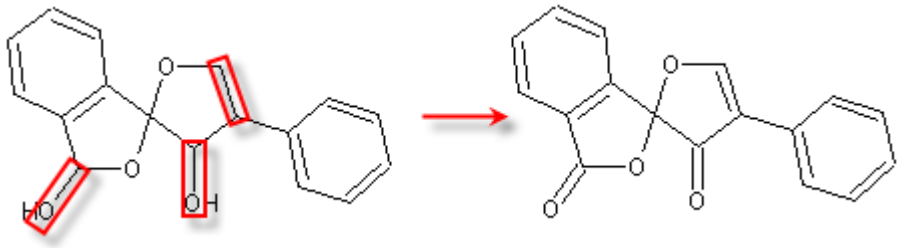
6. On the Atoms toolbar, click **Oxygen** (note that the **Draw Normal** tool is automatically enabled), and then click the indicated carbon atoms to replace them with oxygen atoms:



7. Right-click to quickly switch to the **Draw Continuous** tool, and then double-click the indicated carbon atoms to attach the OH groups to them:



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



> **Note** The CHAPTER5.SK2 file (Page 1/4) with this structure can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

9. On the General toolbar, click **Save File**, in the **Save Document As** dialog box that appears, specify the name and location of the file to which the work should be placed, and click **Save**.

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

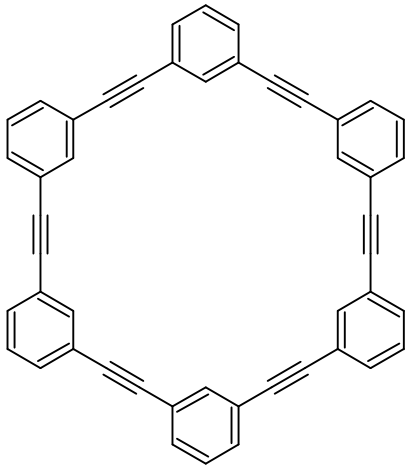
5.4 Instant Template Tool

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 junction point.

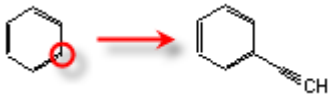
5.4.1 Creating Structure of Cyclic Oligomer

This section is based on the OLIGOMER.EXE movie which can be found in the \\MOVIES\CHEMSK folder.

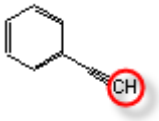
We will draw the following cyclic oligomer structure using templates taken from the Table of Radicals:



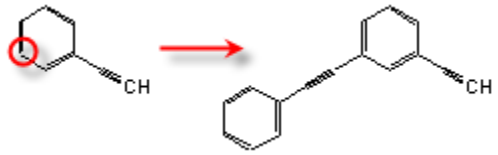
1. On the References toolbar, choose **Benzene**, and click in the upper middle part of the workspace to place a benzene ring.
2. On the References toolbar, click **Table of Radicals**, choose **Ethynyl** C≡CH, and then click the indicated atom to attach it to the ring:



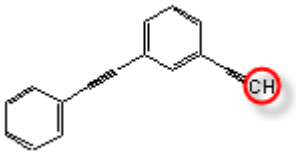
3. On the Structure toolbar, click **Instant Template**, and then click the indicated carbon atom of the triple bond to create an instant template of the drawn fragment:



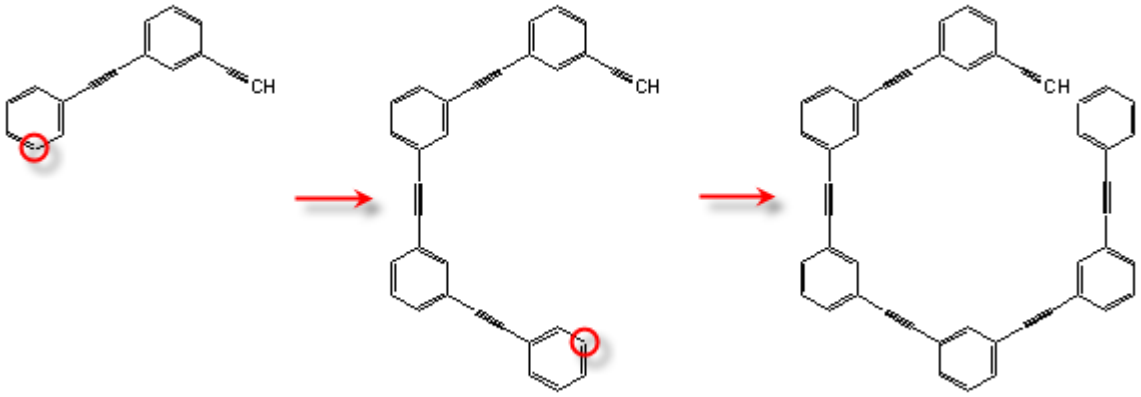
4. Click the indicated carbon atom to attach the template to it:



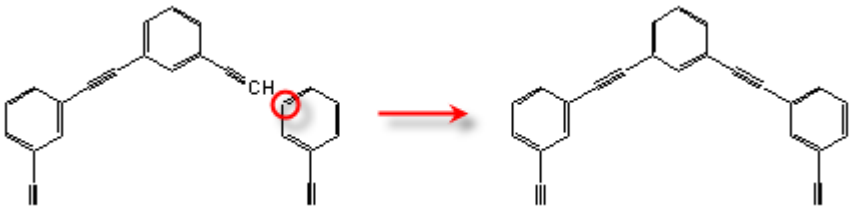
5. Click **Instant Template**  again, and click the indicated carbon atom of the triple bond to create a template of the new fragment:



6. Click the indicated carbon atoms of benzene rings to attach the template as shown:



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



> **Note** The CHAPTER5.SK2 file (Page 2/4) with this structure can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

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

5.5 Template Window

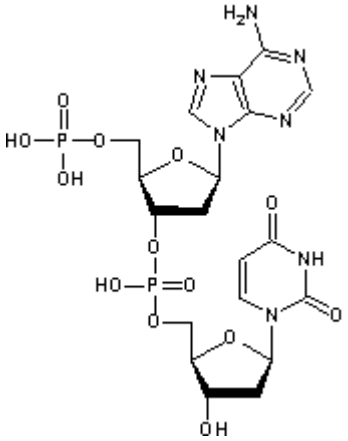
The Template Window feature is the most sophisticated of the three template facilities in ACD/ChemSketch because it allows you to organize and store structures or drawings that you might want to copy later.

A brief tour of available ACD/ChemSketch Templates is given in the TEMPLATE_W.EXE movie which can be found in the \\MOVIES\CHEMSK folder.

5.5.1 Creating Fragment of DNA

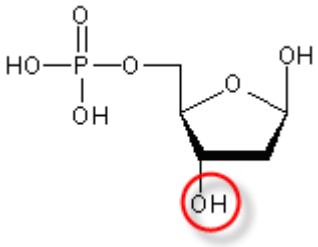
This section is based on the DNA_ST.EXE movie which can be found in the \\MOVIES\CHEMSK folder.

Let's draw the following fragment of single-stranded DNA molecule:



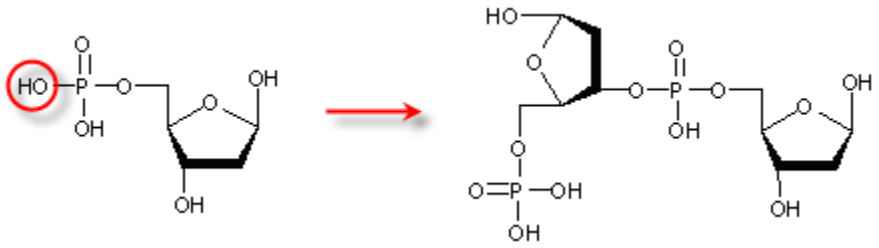
5.5.1.1 Drawing Chain of Deoxyriboso-5-phosphate Fragments

1. On the General toolbar, click **Open Template Window** .
2. On the DNA/RNA Kit tab of the **Template Window** dialog box, choose a structure of *2-deoxyriboso-5-phosphate* (chain form) by clicking the hydroxyl group indicated below to set the point of template's junction:



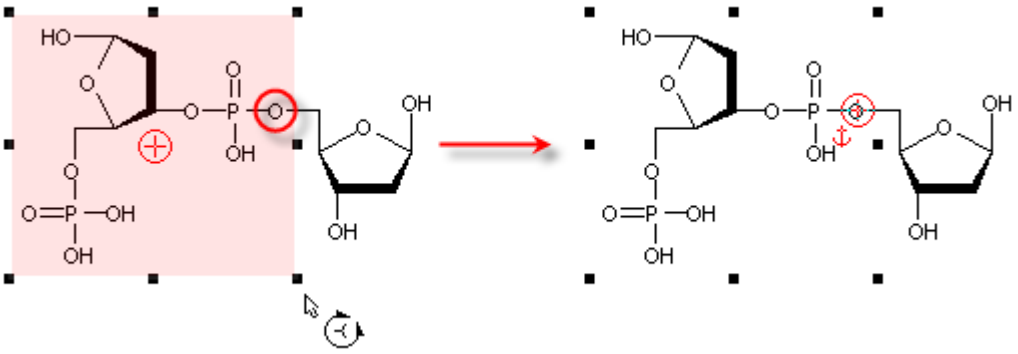
3. Click within the workspace to paste the chosen template.

4. Holding down SHIFT, point to the indicated atom, and click to attach the next *2-deoxyriboso-5-phosphate* fragment:



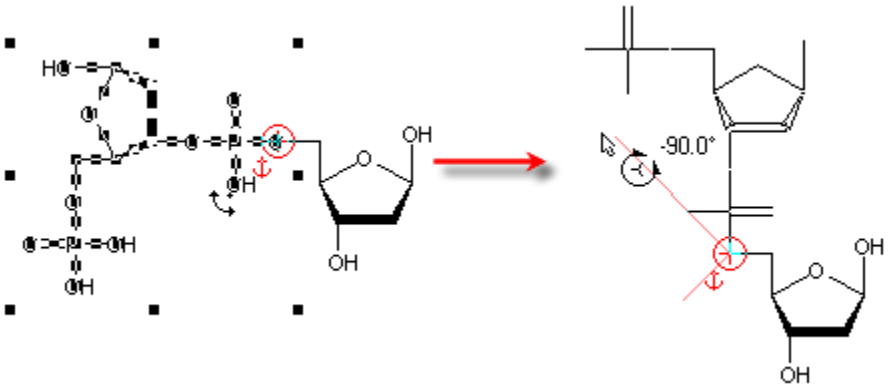
5. Click **Select/Rotate/Resize**  .

6. Drag to select the indicated part of structure, and then drag the action center ⊕ onto the indicated oxygen atom:

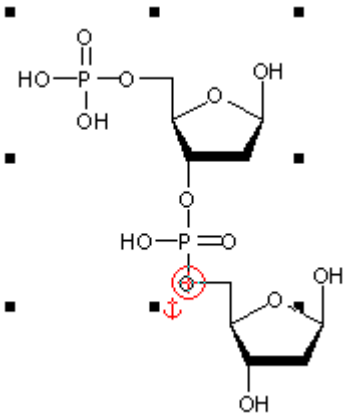


.

7. Holding down SHIFT, point to the fragment to make it selected (note that the mouse pointer is changed to ↻), and drag the selected part of structure clockwise to rotate it by 90°:



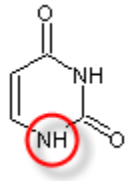
As you release the mouse button, you will see the results of the fragment's rotation:



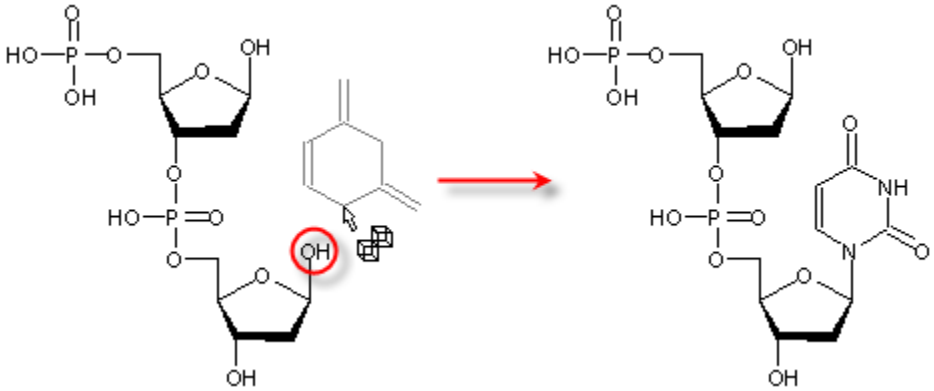
8. Click out of the structure to cancel selection of the fragment.

5.5.1.2 Adding Bases

1. Open the **Template Window** dialog box.
2. On the DNA/RNA Kit tab, choose *uracil* by clicking the indicated nitrogen atom so that this will serve as the attachment point:

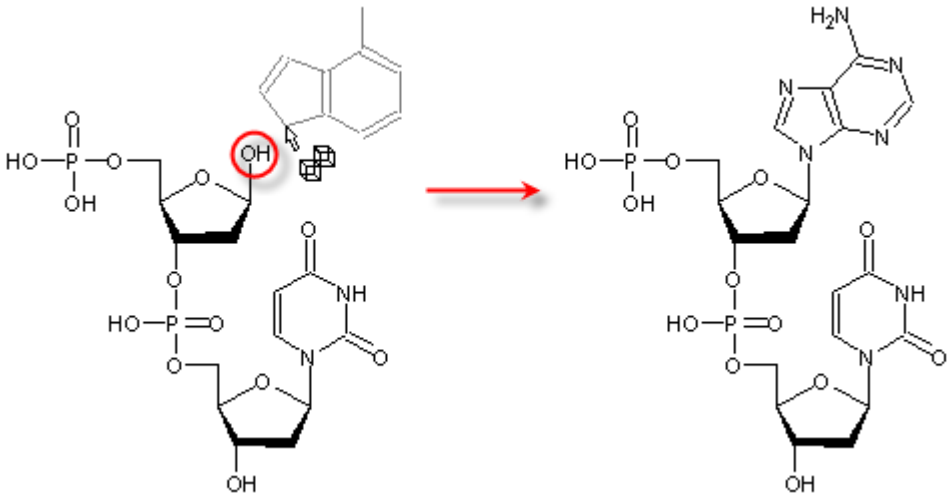


3. Point to the atom indicated below, and click while holding down SHIFT:



> **Tip** You can flip the template's outline before fixing it by pressing TAB.

4. Repeat steps 1 and 2 to add the *adenine* base to the structure:



> **Note** The CHAPTER5.SK2 file (Page 3/4) with this structure can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

5. Now, try to draw your own DNA or RNA fragments of any other length.
6. On the General toolbar, click **Save File**  , then click **New Page**  .

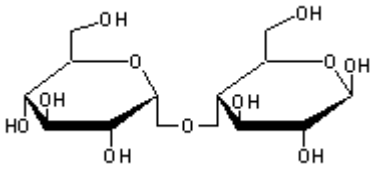
5.6 Drawing Complex Structures of Biomolecules

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

5.6.1 Creating Structure of Beta-Maltose

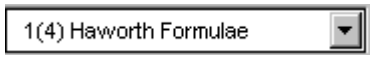
 This section is based on the MALTOSE.EXE movie which can be found in the \\MOVIES\CHEMSK folder.

Let's draw the following structure of *β-Maltose* using templates taken from the Template Window:



1. Open the **Template Window** dialog box, switch to the 

tab, and ensure that you are viewing the Haworth formulae page. If not, select it by choosing the name from the corresponding list at the top of the dialog box:

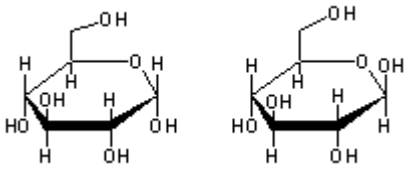


2. Click the structure of *α-D-Glucopyranose* to select it, and click within the workspace to paste it.

3. Repeat steps 1–2, but this time select the Sugars: beta-D-Pyr tab, and choose structure of *β-D-Glucopyranose*.

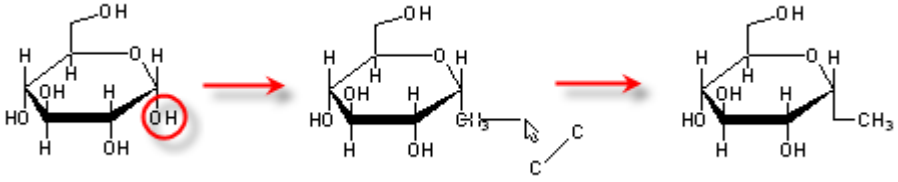
   Note If the **Sugars: beta-D-Pyr** tab is absent at the left part of the dialog box, choose its name from the leftmost drop-down list at the top of the dialog box.

4. Click in the ChemSketch window to place it to the right of the first structure:

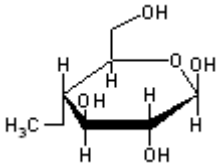


5. On the Atoms toolbar, click **Carbon** C.

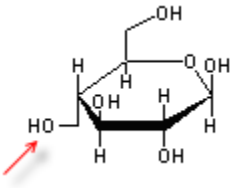
6. Click the indicated atom in the *α-D-Glucopyranose* structure to replace it with a CH_3 group, and then drag from the methyl group to the right while holding down SHIFT to draw the new bond exactly at the right angle:



7. Repeat the previous step for the *β-D-Glucopyranose* structure to obtain the following structure:

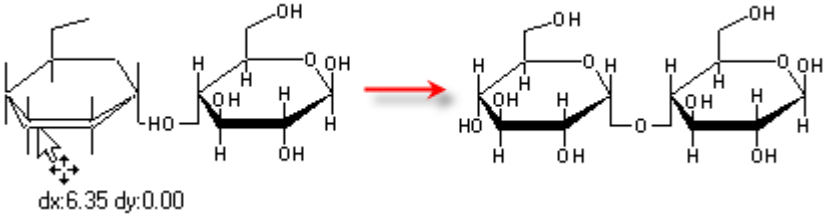


8. On the Atoms toolbar, click **Oxygen** O, and then click the methyl group in the *β-D-Glucopyranose* structure to replace it with the hydroxyl one:



9. On the Structure toolbar, click **Select/Move**. Click in the workspace near to, but not touching, the left *α-D*-structure to select it.

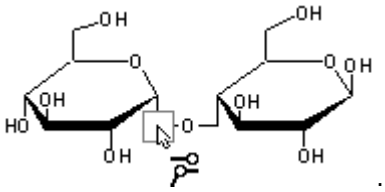
10. Point to any atom or bond of the selected structure, and drag it to the right until the corresponding OH and CH_3 groups overlap each other as shown below, then release the mouse button and click outside the selection:



11. From the **Tools** menu, choose **Remove Explicit Hydrogens** to hide single hydrogens in the selected structure.
12. Through the drawn CH_2 groups in the oxygen bridge are hidden, they are actually present in the structure. If the chemical meaning is important for your task (for example, in calculating the formula weight), you can remove these atoms in one of the following ways:

    a Click **Pseudo Atom** on the **Atoms** toolbar. If this button is missing, click the white bottom right triangle of the displayed **Radical Label** button, and then, on a set of tools that appears, click .

    b Point to the atom group you want to remove, and then click. The CH_2 group will disappear:



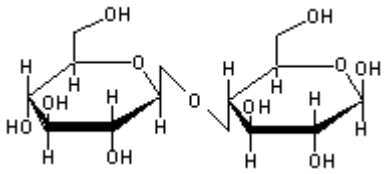
    –OR–

    a With the **Select/Move** tool active, double-click the hidden atom group. The **Properties** panel will appear.

    b Click **Atom Symbol** C, and then, from the adjacent **Value** list, choose **Empty**.

    c Click **Apply**, and then close the panel.

13. Using the technique described above, try to draw the following structure on your own (note that you need to drag at an acute angle in the step 6):



β-Cellobiose

> **Note** The CHAPTER5.SK2 file (Page 4/4) with these two structures can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

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

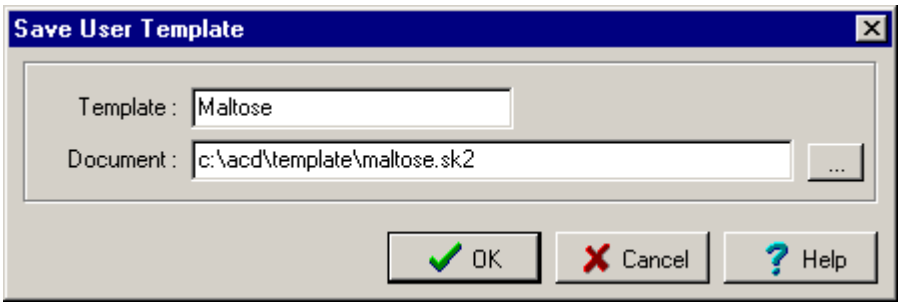
5.7 Defining a User Template

It is very easy to create a template out of a ChemSketch file. We are offering free templates included with the ACD/ChemSketch installation package (the \\TEMPLATE folder).

> **Note** 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 structures you have drawn as a user template:

1. From the **Templates** menu, choose **Save User Template**.
2. If the ChemSketch document has not yet been saved, the **Save Document As** dialog box appears where you can specify the name and location of the file, *e.g.*, C:\ACD\TEMPLATE\MALTOSE.SK2, and click **Save**.
3. In the **Save User Template** dialog box, type the name for your template, such as *Maltose*:



4. Click **OK**.

> **Note** You can enter any name for your template (*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** dialog box (for more information, refer to Section 5.5).

5. Close the active ACD/ChemSketch document.

5.7.1 The User Template Window Organizer

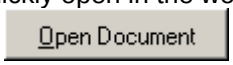
The User Template Window Organizer is a very convenient way for managing template files: both of those included with the software package, and those that you decide to create. It will just take you a moment to add your ACD/ChemSketch document to the list of templates even if the document is closed:

1. From the **Templates** menu, choose **Template Organizer** to display the **User Template Window Organizer** dialog box, and click **New** 

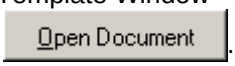
.

2. In the **Create User Template** dialog box, specify the name and location of the needed document, assign a template name to it, and click **OK**.

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 User 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 User 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.
- You can quickly find a document by previewing its contents in the Preview area of the **Template Window** dialog box.
- You can quickly open in the workspace a selected document from the list by clicking **Open Document**  in the **User Template Window Organizer** dialog box.
- Up to 5 user templates can be accessed through the Template Window.

You can perform the following actions with a user template:

⇒ ***Modify a template***. To do this, from the **Templates** list of the User Template Window Organizer, choose the needed template, and click **Open Document**  . Make changes as needed, and then save.

⇒ ***Copy and paste any structure/image of a template to the workspace*** (either Structure or Draw mode) without opening the whole document. To do this, choose your template in the Templates list of the Template Window, and click the item to select it and place to the workspace.

5.7.2 The TEMPLATE.CFG File

The key to management of the templates in ACD/ChemSketch is the TEMPLATE.CFG file. 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 obtain information on 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 (as described above).

If TEMPLATE.CFG is moved or lost, the Template Window will not display any templates. If the TEMPLATE.CFG file can be found (for example, by Windows Explorer or the system's Find File utility), it can be restored either to the default directory or to 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.

6. Calculating Macroscopic Properties

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.

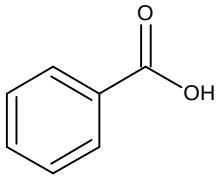
> **Note** Prior to performing any of the procedures described below, ensure that you are in the Structure mode of ACD/ChemSketch.

6.2 Calculating Physicochemical Properties for a Structure

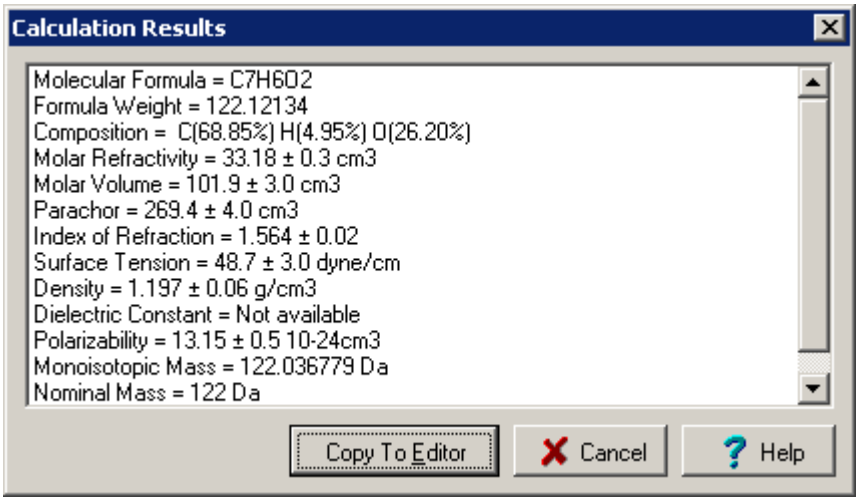
6.2.1 Calculating Properties and Pasting Results to ChemSketch Page

To determine all (or some) of the available physicochemical properties for entire structure, follow the steps:

1. 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). As a result, 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:



3. Click **Copy to Editor**  to paste the results in the workspace. As the text is inserted, you are switched to the Draw mode where you can 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.

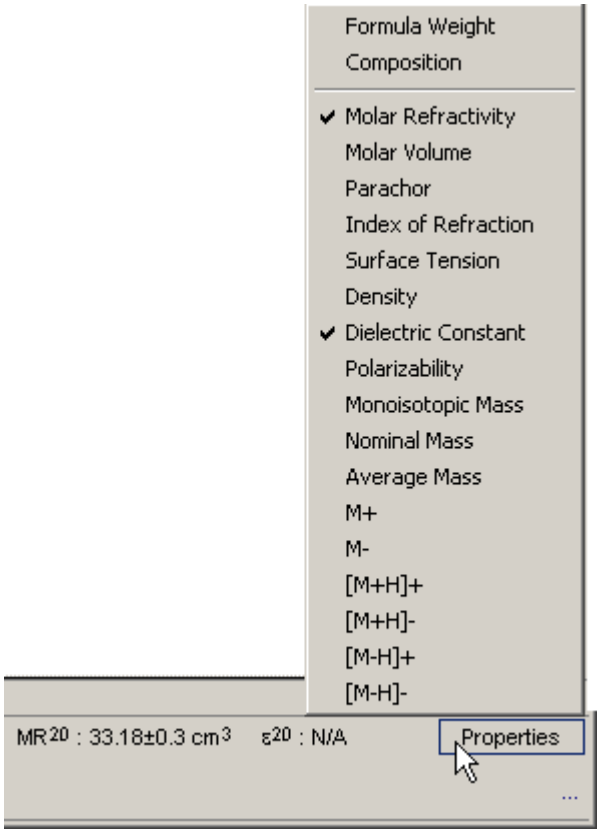
4. Switch back to the Structure mode and save the document to CALC_PROP.SK2.

> **Note** The CHAPTER6.SK2 file (Page 1/2) with the structure and calculation results can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

6.2.2 Displaying Properties Automatically on Status Bar

It is also possible to view the physicochemical properties for the structure selected in the workspace directly on the status bar:

- On the status bar, click **Properties** Properties, and repeatedly choose the desired properties from the menu by placing ticks next to the corresponding properties' names:



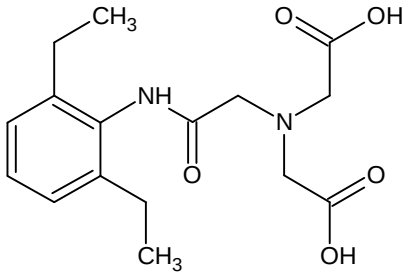
> **Note** If no structure is selected in the workspace, the properties are calculated for all the structures displayed; if there are no structures drawn, no properties will be displayed.

By default, the display of the properties is set to formula weight. In the example shown, the molar refractivity, MR^{20}: 33.18±0.3 cm^3, and dielectric constant, ε^{20}, have been specified.

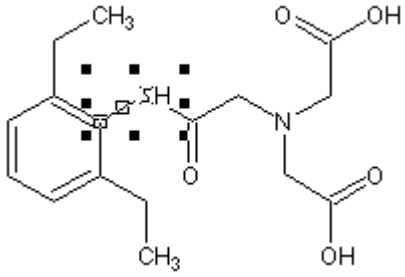
6.3 Calculating Monoisotopic Mass for a Fragment (MassSpec Scissors)

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

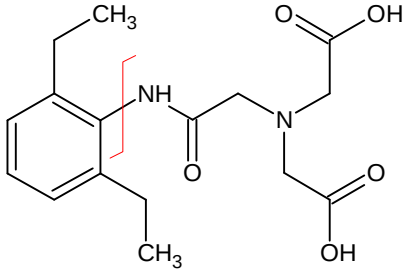
1. On the General toolbar, click **New Page**  to add a new blank page in current ACD/ChemSketch document.
2. Draw a structure—for example, the following acid:



3. Select a bond to cut (it should be a non-cyclic one):



4. From the **Tools** menu, choose **MassSpec Scissors** (or click the corresponding **MassSpec Scissors**  button on the Structure toolbar). This will display monoisotopic mass underneath BOTH of the structural fragments in the workspace:



$C_{10}H_{13}$ $C_6H_9N_2O_5$
133.1017 Da 189.0511 Da

You can change the style of the separating line: in the Draw mode, double click the line, and then, on the **Objects Panel** dialog box, change the style as desired.

You can also see the nominal and average masses on the status bar using the **Properties** Properties tool (refer to Section 6.2.2).

> **Note** The CHAPTER6.SK2 file (Page 2/2) with this structure can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

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

7. Special Function Keys

7.1 Objectives

ACD/ChemSketch is an extremely versatile molecular structure editor. For this reason, several ACD/Labs modules are 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 Add-On are included with both commercial and freeware versions of ACD/ChemSketch; ACD/Dictionary is also available but only with the commercial software.

> **Note** Prior to performing any of the procedures described below, ensure that you are in the Structure mode of ACD/ChemSketch.

7.2 ACD/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 the **Check for Tautomeric Forms**  button on the Structure toolbar.

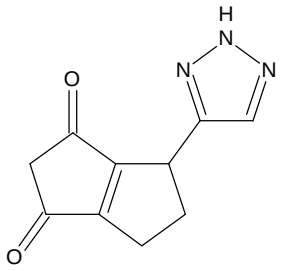
The possibility of the alternative tautomeric forms should always be carefully considered, if the drawn organic structure contains two or more double or triple bonds conjugated with or attached to oxygen, nitrogen, sulfur, or other heteroatoms. The current ACD/Tautomers algorithm provides only the suggested 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.

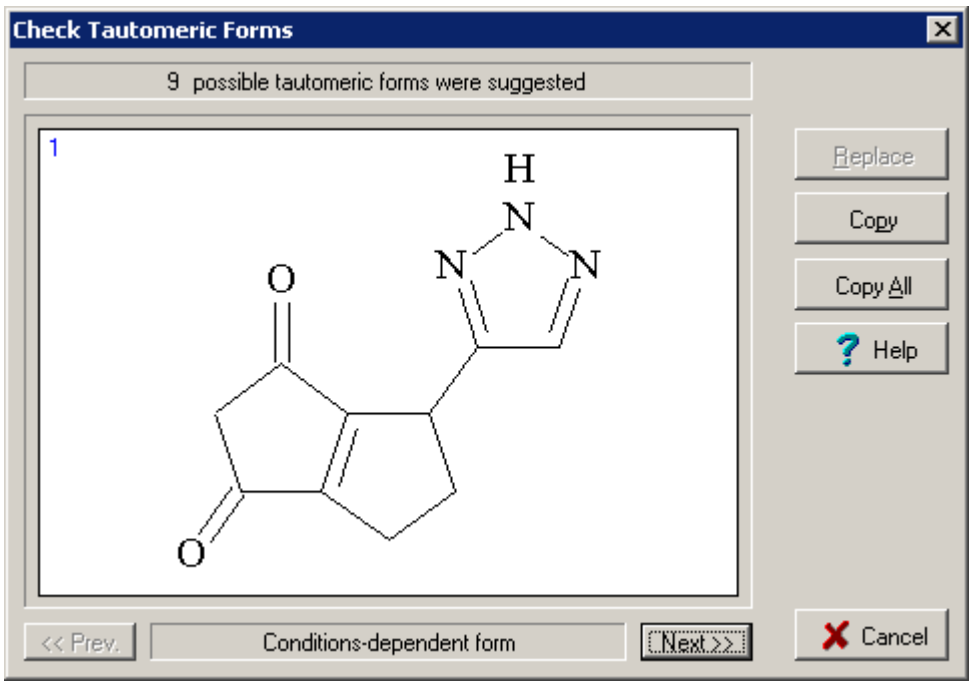
Now we are going to try this option on the illustrative example:

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



> **Note** The CHAPTER7.SK2 file with this structure can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.

2. Select the structure, and then, 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:

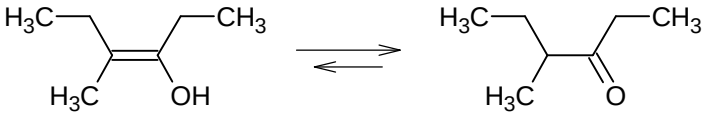
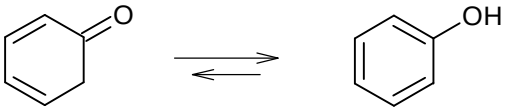
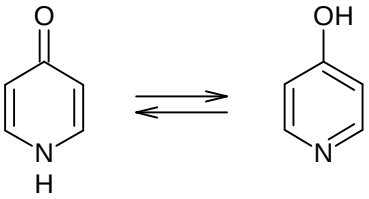
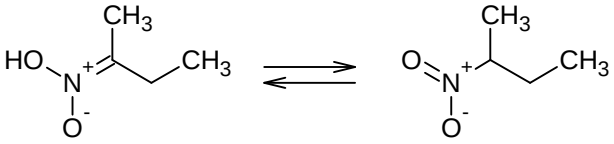
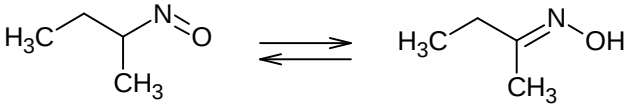
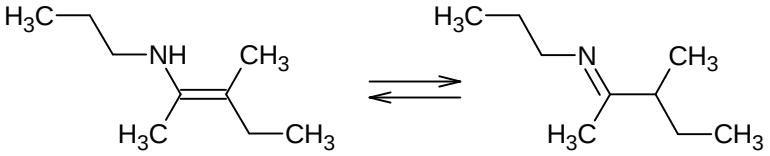


3. Using the **Next >>** or **<< Prev** buttons, select the second tautomeric form (*4-(2H-1,2,3-triazol-4-yl)-5,6-dihydropentalene-1,3(2H,4H)-dione*).

4. Click **Replace**  to change the drawn structure for the currently selected one.

7.2.1 Examples

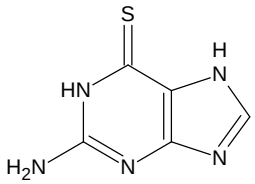
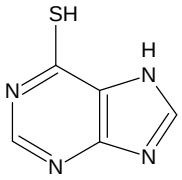
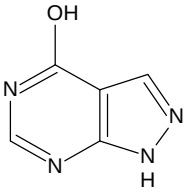
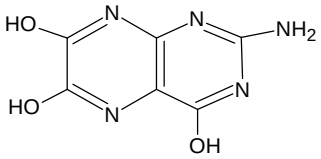
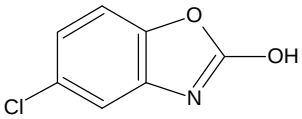
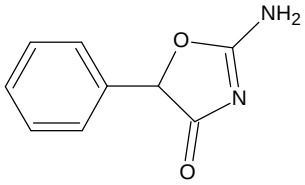
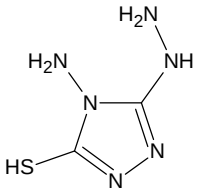
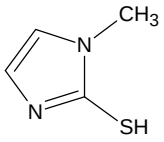
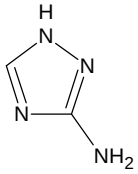
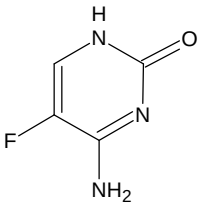
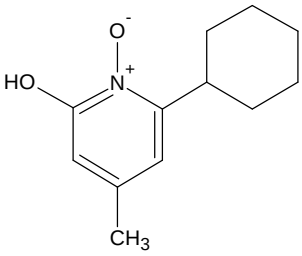
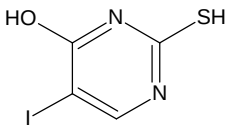
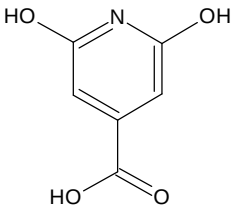
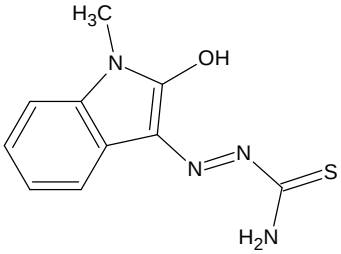
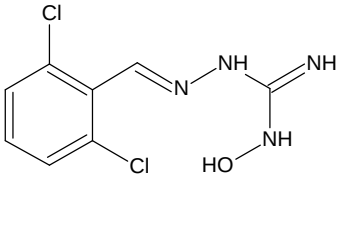
Here are a few “classic” types of tautomerism which you can try out with the Check Tautomeric Forms feature described above.

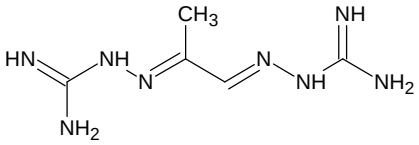
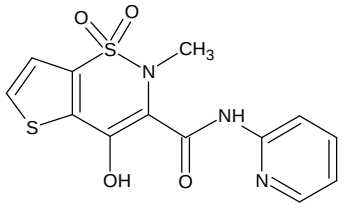
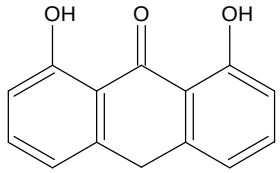
Tautomerism	Example
Keto-Enol	
Phenol-keto	
Heterocyclic ring	
Nitro-acid form	
Nitroso-oxime	
Imine-Enamine	

7.2.2 Mistakes in 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 (antiurolithic) 6 possible forms
		
Leucopterin >10 possible forms	Chlorzoxazone (skeletal muscle relaxant) 2 possible forms	Pemoline (CNS stimulant) 3 possible forms
		
Purpald 4 possible forms	Methimazole (antihyperthyroid) 2 possible forms	Amitrole (herbicide) 5 possible forms
		
Flucytosine (antifungal) 6 possible forms	Ciclopirox (antifungal) 2 possible forms	Iodothiouracil (thyroid inhibitor) 6 possible forms
		
Citrazinic acid 2 possible forms	Methisazone (antiviral) 2 possible forms	Guanoxabenz (antihypertensive) 3 possible forms

Questionable Structures from Various Publications		
		
Mitoguazone (antineoplastic) >10 possible forms	Tenoxicam (anti-inflammatory, analgesic) 4 possible forms	Anthralin (antipsoriatic) 2 possible forms

7.3 ACD/Dictionary

For Commercial Version only

ACD/Dictionary is an add-in module that is supplied with all of 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 165,000 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.

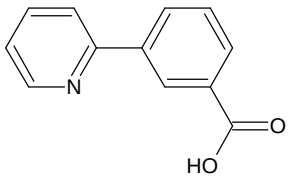
> **Note** If you have purchased ACD/ChemSketch, but do not see the **Dictionary** button  on the References toolbar when you are in the Structure mode, please verify that you have correctly entered TWO registration numbers at the time of installation by checking them in the List of Registration Keys of the ACD/Labs Registration dialog box (\\REGISTER.EXE): the one for ACD/ChemSketch (Main), and another for the ACD/Dictionary (Add-in).

7.4 ACD/Name Freeware Add-on

Within the ACD/ChemSketch, it is possible to use ACD/Name Freeware Add-On. This extra functionality is available via either the **Generate Name for Structure** button  on the General toolbar or the **Generate>Name for Structure** command from the **Tools** menu.

This tool is easy to use, so let's try naming some example structures to demonstrate this:

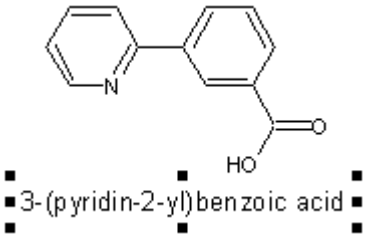
1. Using ChemSketch tools, draw the following structure:



2. If there is more than one structure drawn in the workspace, select only the above structure.

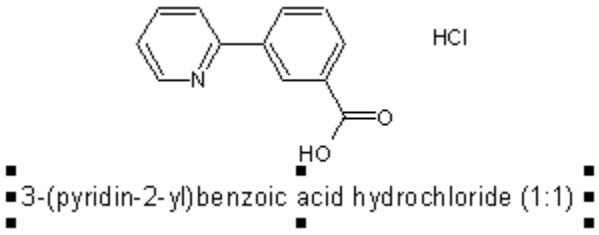
> **Note** If no specific structure is selected, the program will generate chemical names for ***all*** of the structures found in the workspace, considering them as a mixture of compounds in a corresponding proportion.

3. On the General toolbar, click **Generate Name for Structure**  . The name appears selected below the drawn structure:



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

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



> **Note** The CHAPTER7.SK2 file with this structure can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.

7. Click somewhere in the workspace to cancel selection of the name string.
8. Save your work as the EXAMPLE4_1.SK2 file.

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/draw_nom/nom/name/**

8. Searching for Structures—Commercial Version Only!

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.

> **Note** Prior to performing any of the procedures described below, ensure that you are in the Structure mode of ACD/ChemSketch.

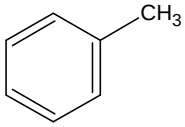
8.2 Searching for Structure

The Search for Structure tool 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.

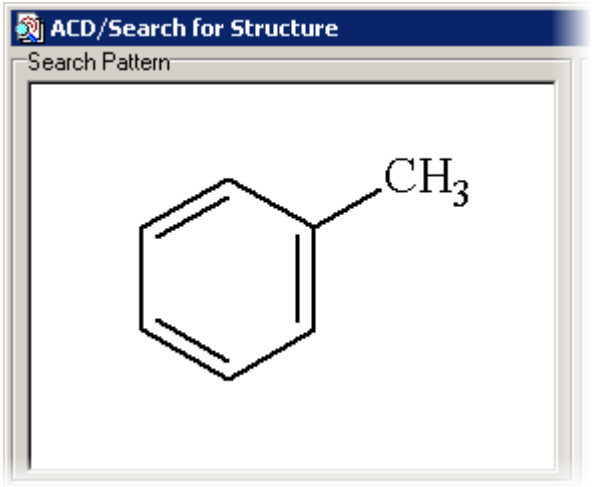
8.2.1 Specifying Files to Search Through

You can search for specific structures through the files of currently available formats:

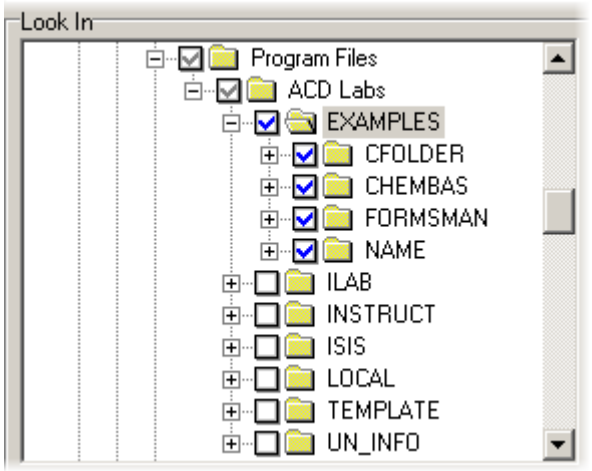
1. On the General toolbar, click **New Page**  .
2. Draw a structure of *toluene* (or find it in ACD/Dictionary):



3. On the General toolbar, click **Search for Structure** to display the **ACD/Search for Structure** dialog box. Note that the drawn structure is placed to the **Search Pattern** box:

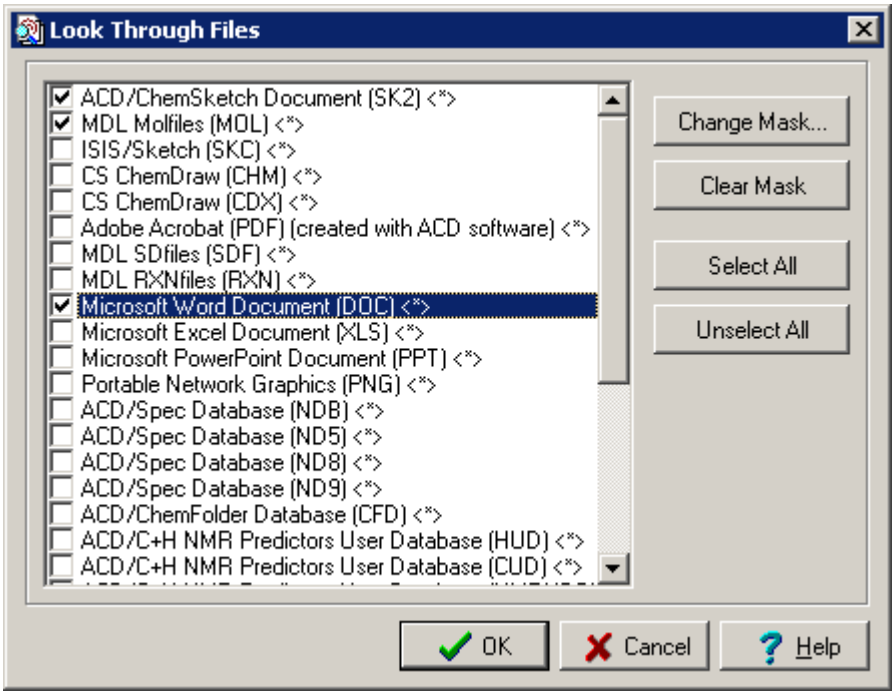


4. In the **Look In** box, select the folders and/or files to search through. For our example, find the ACD/Labs example folder and select it with all of the subfolders:



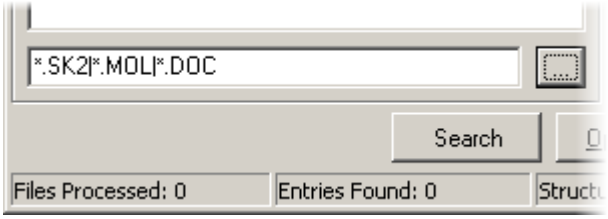
5. To set the formats of the files to search through, click **Browse** ... below the **Look In** box to display the **Look Through Files** dialog box.

6. Click **Unselect All**  to clear all of the check boxes, and then select the **ACD/ChemSketch Document**, **MDL Molfiles**, and **Microsoft Word Document** check boxes:



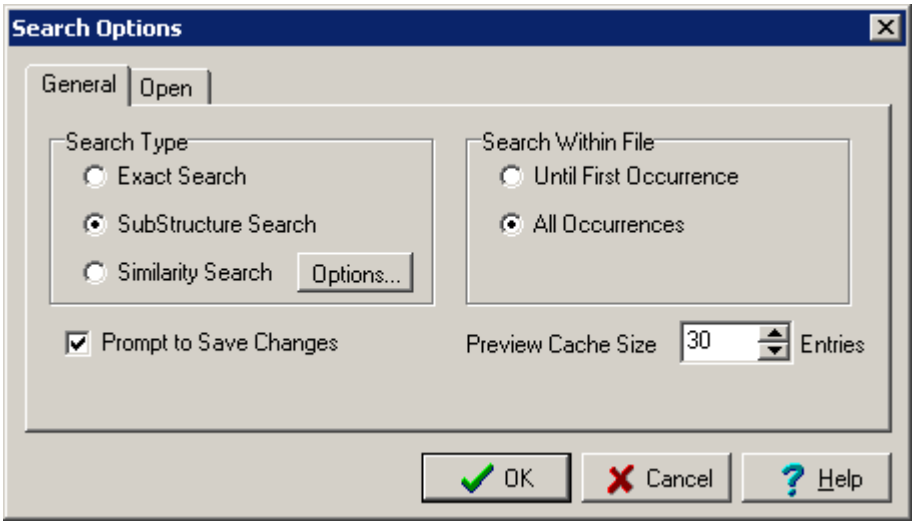
> **Tip** You can narrow the search by defining the file mask for any of the selected formats: highlight the format name in the list, then click **Change Mask**  , and type a file mask in the dialog box that appears.

7. Click **OK** to apply your changes:



8. In the **ACD/Search for Structure** dialog box, click **Options** 

to display the **Search Options** dialog box:

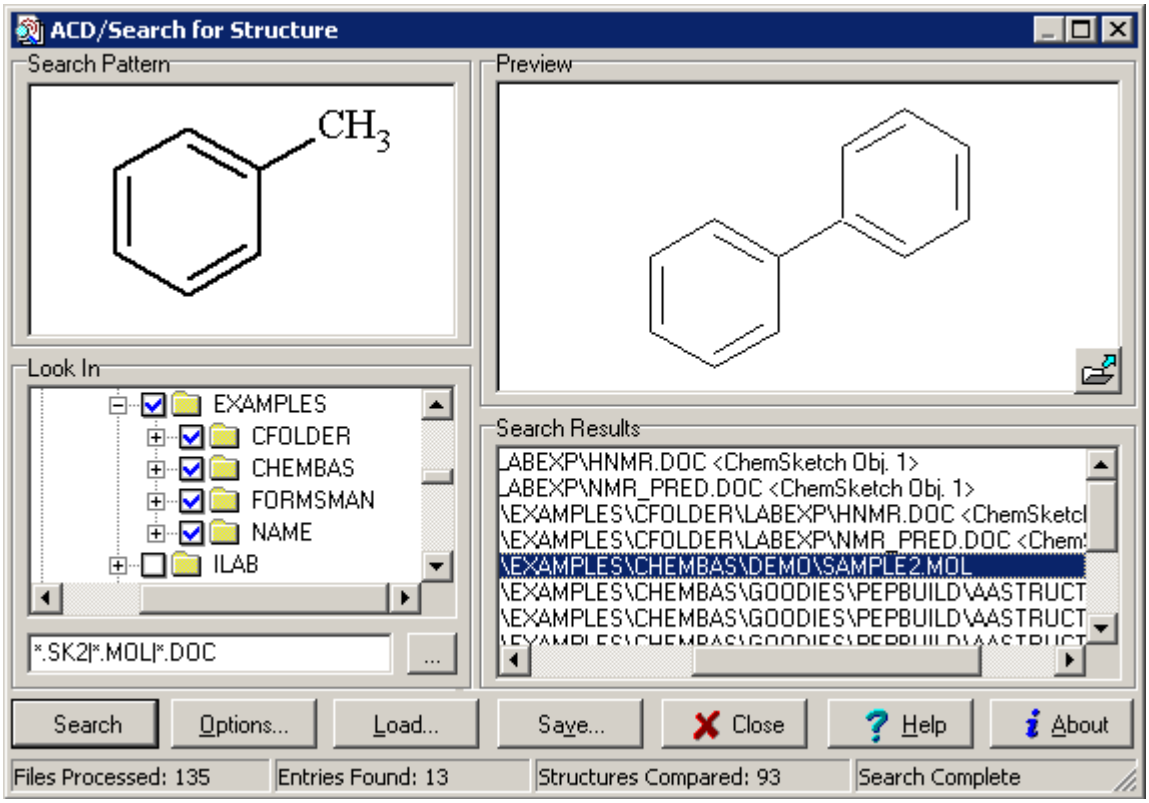


9. On the **General** tab, under **Search Type**, choose **SubStructure Search**, and then, in the **Search Within File** area, choose **All Occurrences**.
10. Switch to the **Open** tab, and define the application to be used for opening the corresponding files—for this example, leave the default **Open in ChemSketch** option selected.
11. Click **OK**.

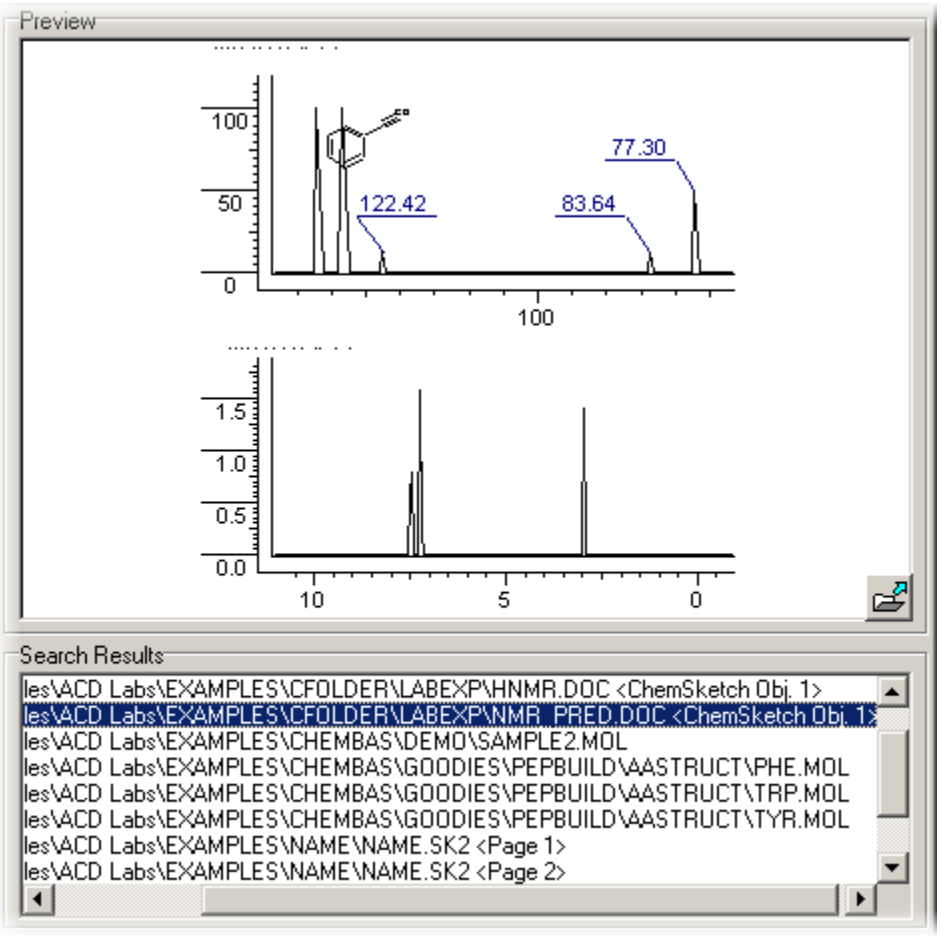
8.2.2 Considering Search Results

Now, we can perform search for the desired substructure:

1. In the **ACD/Search for Structure** dialog box, click **Search** Search. As the search proceeds (note that during this the **Search** Search tool changes to the **Stop** Stop one), pathnames of the files where the query structure is found are displayed in the **Search Result** area of the dialog box.
2. Click the desired name in the list of found files to view the structure(s) found by your query in the **Preview** area:



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



To open the found file, in the **Preview** area, click **Open** or double-click the file name in the **Search Results** list.

To save the search results, as well as the query structure and folder settings, into an ACD/Search for Structure file (.SSF), click **Save** Save... . Thereafter, you can open this file by clicking **Load** Load... .

> **Note** If a found .SK2 file is opened in ACD/ChemSketch, a new page is created, in other cases, the file opens as usual.
> As the opening takes place, you do not leave the **Search for Structure** dialog box.

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

9. Creating Graphical Objects

9.1 Objectives

This chapter will familiarize you with the creation of graphical objects in the Draw mode of ACD/ChemSketch. You will learn how to use the 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.

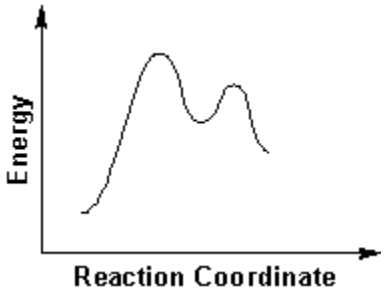
You will also learn how to output PDF files, a task that can be done for graphical or chemical objects.

> **Note** Prior to performing any of the procedures described below, ensure that you are in the Draw mode of ACD/ChemSketch.

9.2 Drawing the Energy of Reaction Diagram

 This section is based on the DIAGRAM.EXE movie which can be found in the \\MOVIES\CHEMSK folder.

We are going to draw the following diagram:



9.2.1 Drawing a Curve

With the Polyline tool, you can create a curve (*Bézier curve*) by adding a node (*anchor point*) where a curve changes direction, and dragging the direction lines that shape the curve. The length and slope of the direction lines determine the shape of the curve.

This section describes how to draw a curve:

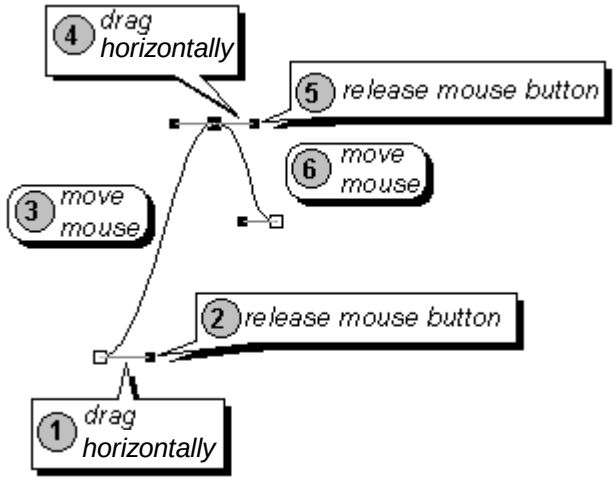
1. On the General toolbar, click Draw to switch to the Draw mode of ACD/ChemSketch.
2. From the **File** menu, choose **New** to start a new document.
3. On the Drawing toolbar, click **Polyline** .
4. Position the Polyline tool where you want the curve to begin, and drag horizontally to the right from the starting node of the curve to extend the direction line (as shown step-by-step in the picture below).

   > **Tip** In general, extend the direction line about one third of the distance to the next node you plan to place. By changing the length of the lines you can modify the curve segment. You can adjust one or both sides of the direction line later (for more information, refer to the following section).

5. Release the mouse button.
6. Move the mouse up to the point where you want the first curve segment to end.
7. Drag horizontally to the right to extend the direction line.

   > **Note** To create a C-shaped curve, drag in a direction opposite to the previous direction line.
   > To create an S-shaped curve, drag in the same direction as the previous direction line.

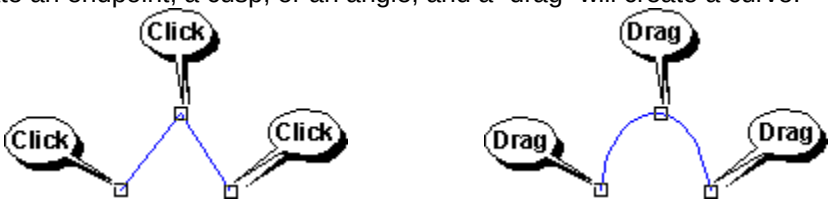
8. Release the mouse button.
9. Move the mouse down to the point where you want the second curve segment to end:



10. Repeat the above steps to draw the next two segments of the curve.

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 an angle, and a "drag" will create a curve:

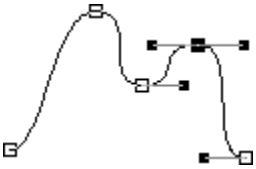


9.2.2 Modifying a Curve

The first time you draw a curve 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. On the Editing toolbar, click **Select/Move/Resize**, and then click the curve to select it.
2. On the Editing toolbar, click **Edit Nodes**. This will show all of the nodes on the curve that can be modified:

3. Click the required node to select the it and view corresponding direction lines:



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

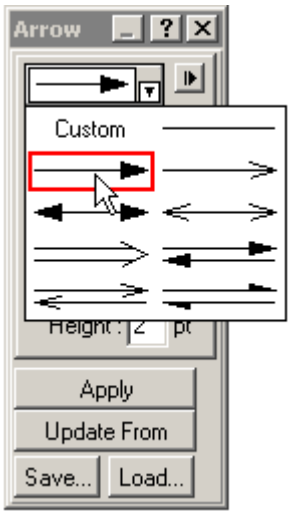
> **Tip** When using the **Edit Nodes** tool, you can manipulate nodes using the buttons on the Node toolbar that appears. For example, you can select several nodes by clicking on them when holding down SHIFT, and then align them by choosing the corresponding button on the toolbar.

9.2.3 Drawing the X and Y axes

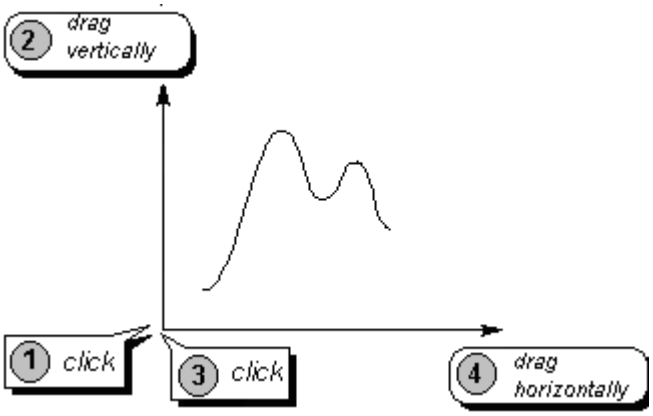
To accomplish drawing of a reaction diagram, the axes are required.

1. On the Drawing toolbar, click the **Arrow** tool.
2. From the **Tools** menu, choose **Arrow Style Panel** to display the **Arrow** panel.

3. From the drop-down list, choose the one-way arrow:



4. Close the panel.
5. From the **Options** menu, select **Snap on Grid** and/or **Show Grid** to make your drawing easier.
6. Position the mouse pointer at the origin of coordinates, and drag the mouse up vertically to draw the Y-axis.
7. Position the mouse pointer at the origin of coordinates, and drag the mouse horizontally to the right to draw the X-axis:



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

> **Note** The CHAPTER9.SK2 file (Page 1/6) with this diagram can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

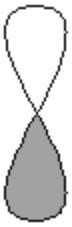
9. From the **Options** menu, deselect **Snap on Grid** and/or **Show Grid**.
10. On the General toolbar, click **New Page**.
11. Save your work as the EXAMPLE5_1.SK2 file.

9.3 Drawing Different Kinds of Orbitals

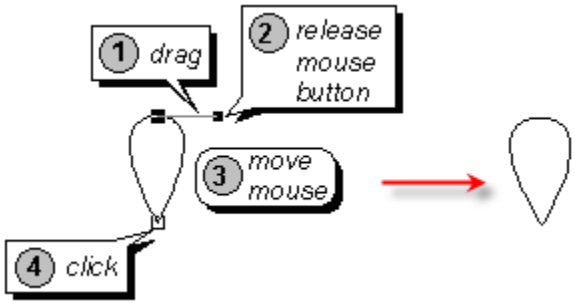
This section explains how to draw three kinds of orbitals: *p*-orbital, *d*-orbital, and *pi*-orbital.

9.3.1 Drawing a *p*-Orbital

We are going to draw the following *p*–orbital:



1. On the Drawing toolbar, click **Polygon**  .
2. Drag horizontally to the right from the starting point to extend the direction line.
3. Release the mouse button.
4. Move the mouse down to draw the body of the half-orbital.
5. Click to fix the half-orbital.
6. Right-click to finish drawing the half-orbital, and then right-click again to quickly switch to the **Select/Move/Resize**  tool:

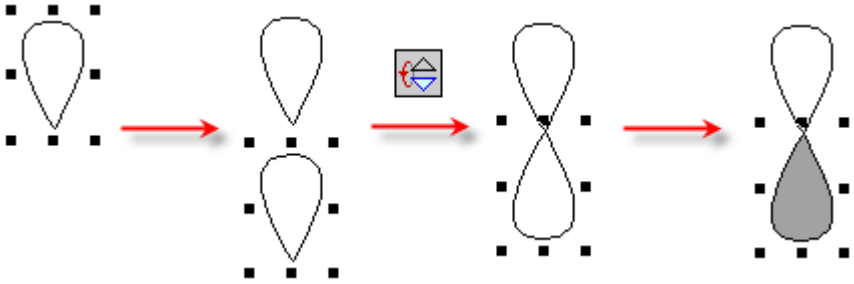


> **Note** If the shape of the curve is not what you want, use the **Edit Nodes**  tool (refer to Section 9.2.2).

7. Point to the selected half-orbital, and drag it down holding down CTRL to make a copy.
8. On the Editing toolbar, click **Flip Top to Bottom**  to flip the lower half-orbital.
9. Put the half-orbitals together by moving them.

> **Tip** To arrange the orbital segments more precisely, make sure that the **Snap on Grid** is not selected on the **Options** menu.

10. Click the gray color on the Color palette at the bottom of the window to change the fill color of the orbital segment:



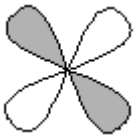
> **Tip** To quickly center the orbital segments, select them both, and click **Center Horizontally**  .

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

> **Tip** You can also choose the orbital template (either large or small) from the set of orbitals available in the **Template Window** dialog box.

9.3.2 Drawing a *d*-Orbital

In this section, we will draw the following *d*–orbital:

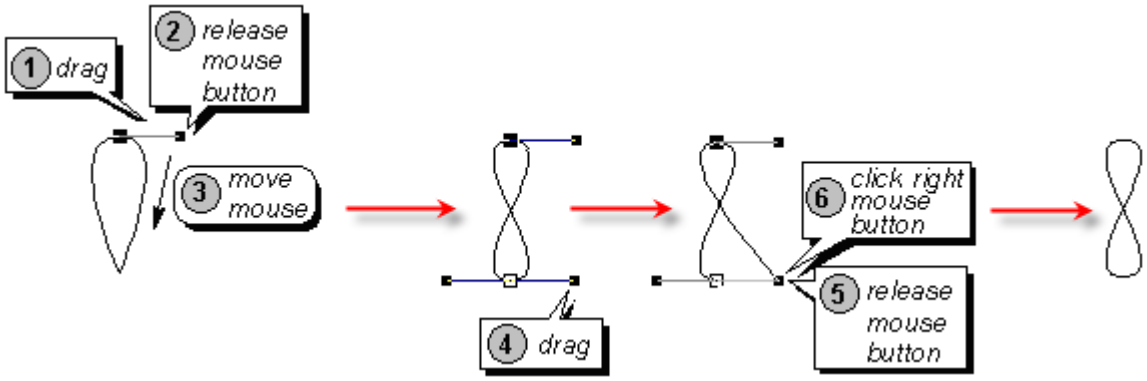


1. Select the **Polygon**  tool again.

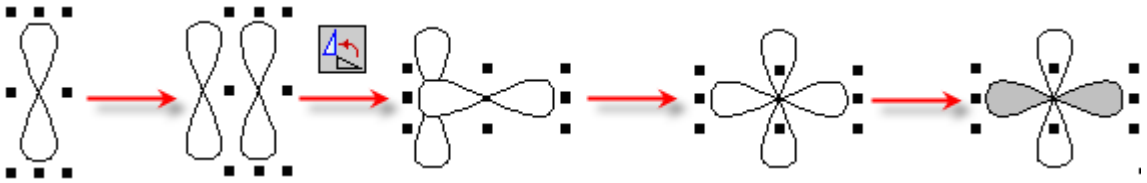
> **Tip** From the **Options** menu, choose **Snap on Grid** before drawing to ease the drawing of the symmetrical orbital.

2. Drag horizontally to the right from the starting point of the orbital to extend the direction line.
3. Release the mouse button.
4. Move the mouse down to draw the body of the half-orbital.
5. Drag horizontally to the right to extend the direction lines. Note that to make the two segments of the half-orbital identical, make the lengths of the direction lines equal.
6. Release the mouse button.

7. Right-click to finish drawing the half-orbital, and then right-click again to switch to the **Select/Move/Resize** tool:



8. With the half-orbital selected and holding down CTRL, drag to make a copy of it.
9. On the Editing toolbar, click **Rotate 90°** to rotate the copy of the half-orbital.
10. Drag the copy as shown below in the picture.
11. Click the gray color on the Color palette at the bottom of the window to change the color of the orbital segment:



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

12. Select both the segments of the orbital, and click **Group** on the Editing toolbar. Now you can manipulate the segments as a single object.
13. On the Editing toolbar, click **Select/Move/Rotate** tool, and then rotate the selected drawing by 45 degrees while holding down SHIFT.

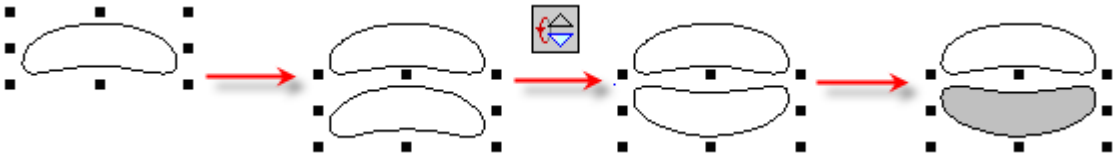
9.3.3 Drawing a *pi*–Orbital

We will draw the following *pi*–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, holding down CTRL, drag down the selected half-orbital to make a copy of it.
6. Click **Flip Top to Bottom** to flip the lower half-orbital, and then move it to an appropriate position.
7. Click the gray color on the Color palette at the bottom of the window to change the color of the orbital segment:



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

8. Select both the segments of the orbital, and click **Group** on the Editing toolbar. Now you can manipulate them as a single object.

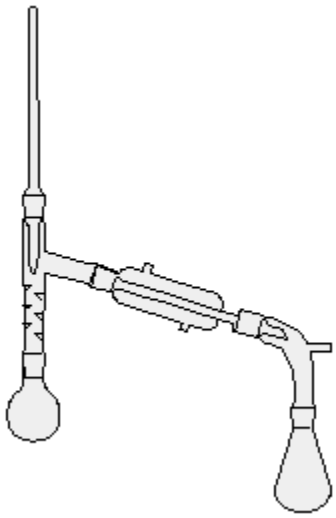
> **Note** The CHAPTER9.SK2 file (Page 2/6) with the orbitals of three different kinds represented in this chapter can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

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

9.4 Drawing Vacuum Distillation Apparatus

This section is based on the APPARAT.EXE movie which can be found in the \\MOVIES\CHEMSK\ folder.

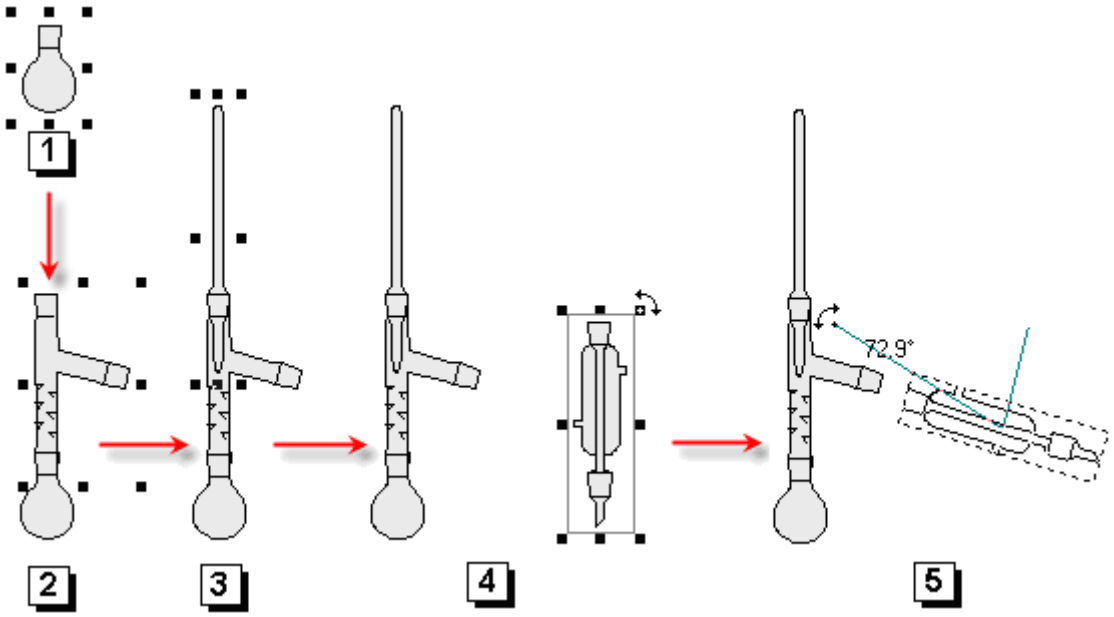
We are going to draw the following apparatus:



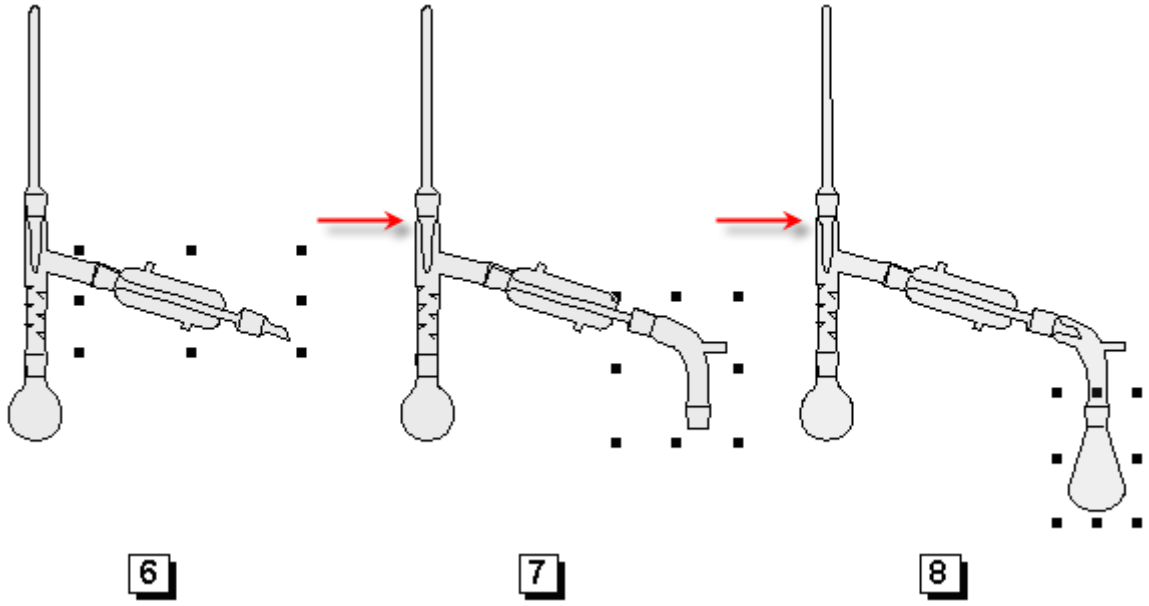
1. From the **File** menu, choose **Page Setup**, and then, on the **Size&Orient.** tab of the dialog box that appears, select **Landscape**. Click **OK** to close the dialog box.
2. On the General toolbar, in the Zoom box, set the zoom value to 50%.

   > **Tip** You can also choose the **Show Grid** and **Snap On Grid** commands from the **Options** menu to activate the grid-snapping mode and facilitate the process of your apparatus assemblying.

3. Click **Template Window** to display the corresponding dialog box, and then, from the list of templates, choose **Lab Kit**.
4. Click the round-bottom flask (refer to the scheme below).
5. Click in the workspace to add the selected template.
6. Open the **Template Window** dialog box. Select the three-way adapter (Vigreux distillation column with connecting adapter). Connect it to the flask by clicking.
7. From the **Template Window** dialog box, choose the thermometer, and connect it by clicking as shown below.
8. From the **Template Window** dialog box, choose the Liebig condenser and place it on the workspace near the apparatus by clicking. Right-click to hide the template's outline and switch to the **Select/Move/Resize** tool.
9. 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° counter-clockwise by dragging any selection handle. The informative cursor will show you the angle of rotation (if the corresponding **Informative Cursor** option has been selected on **General** tab of the **Preferences** dialog box (**Options > Preferences** command):



10. Drag the column, and attach it to the apparatus.
11. From the **Template Window** dialog box, choose the vacuum-distilling adapter, and attach it to the apparatus.
12. With the adapter still selected, click **Send to Back**  to send the selection to the background. This will prevent overlaying of the Liebig condenser's outlet by the adapter template in the drawing.
13. Complete the drawing by connecting the receiving flask (round-bottom flask) taken from the list of templates:

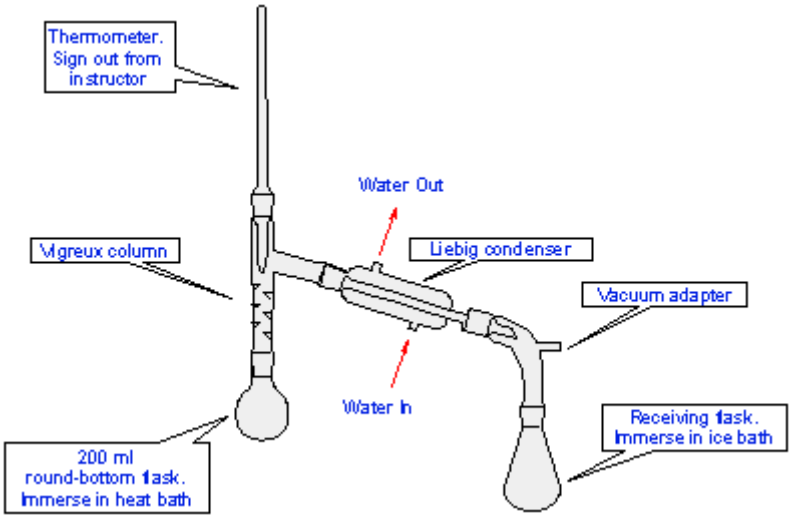


> **Tip** You can also find the complete template of the vacuum distillation apparatus on the second page of the Lab Kit list of templates.

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.

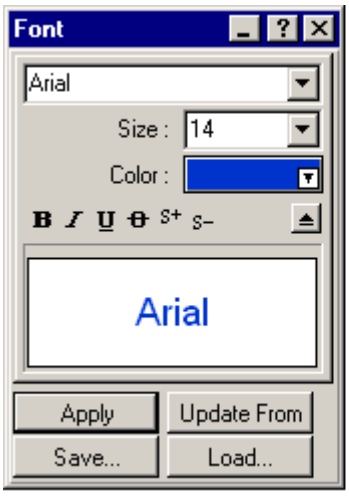
Let's say that you are preparing the diagram for an instruction manual in an undergraduate laboratory. You might want to direct the attention of the students to certain aspects of the set-up, possibly even to remind them what the parts are named, or where they are kept in the lab:

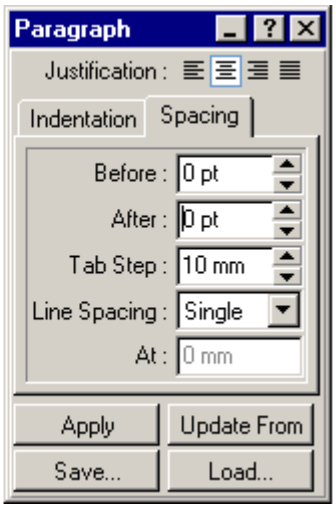


9.4.1.1 Adding Text Captions

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

1. First, let us set the font to be used for the text. From the **Tools** menu, choose the **Font Panel** and **Paragraph Panel** commands.
2. Specify the settings as follows, and then close the panels:





3. On the Drawing toolbar, click **Text**  ,

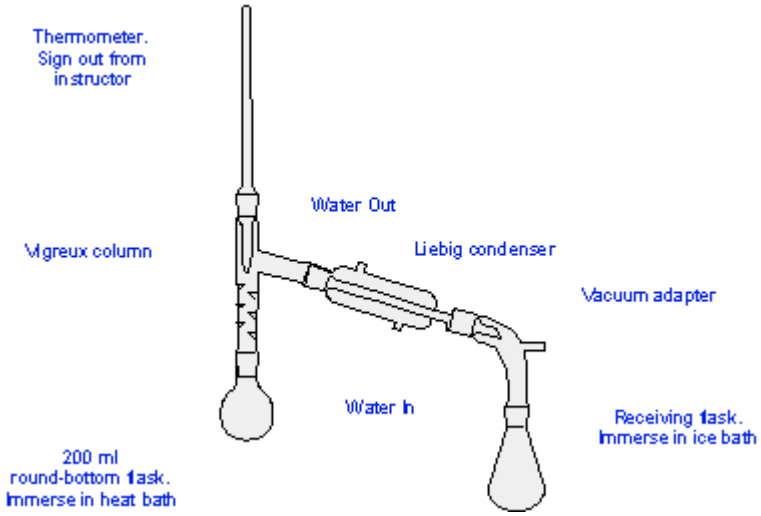
4. Click to the left of the thermometer. In the text box that appears type *Thermometer. Sign out from instructor*. To narrow the text box, drag its right border:

5. 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.

6. Repeat steps 4 and 5 to add other captions.

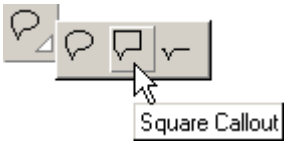
7. If necessary, right-click to quickly switch to the **Select/Move/Resize** tool, and then move the captions to arrange them around the apparatus:



9.4.1.2 Inserting Callouts

Now we are going to include the captions into callouts.

1. On the Drawing toolbar, click the right-bottom corner (*i.e.*, the small white triangle) of the **Callout** button to view the drop-down panel, and choose the square callout type:



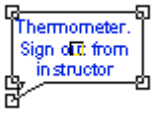
2. Point to the first text caption so the that callout outline appears around it, and click to fix the callout:

3. Subsequently point to other captions (except for ***Water In*** / ***Water Out***), and click to fix the callouts.
4. Right-click in the workspace to leave the Callout mode.

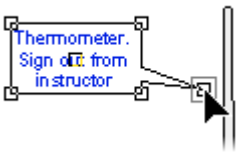
9.4.1.3 Reshaping Callouts

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

1. On the Editing toolbar, click **Edit Nodes**  .
2. Select the first drawn callout by clicking it. Note that the nodes appear on the callout:



3. 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.

4. Without leaving the Edit Nodes mode, click other callouts and repeat step 2.
5. As soon as all the callouts are redirected as necessary, right-click in the workspace to leave the Edit Nodes mode.
6. Using the **Draw Arrow**  tool from the Drawing toolbar, add arrows to indicate the water inlets and outlets.
7. Select both the arrows, and double-click to display the **Objects Panel** dialog box.
8. Set the pen color to red, click **Apply**, and then close the panel.

> **Note** The CHAPTER9.SK2 file (Page 3/6) with the distillation apparatus can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

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

9.5 Drawing a Two-chain DNA Strand

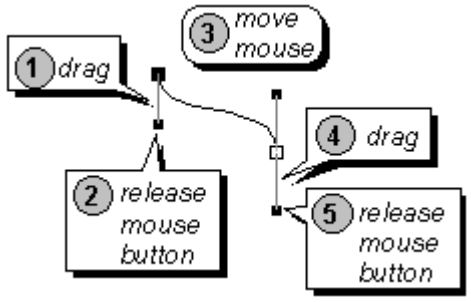
This section is based on the DNA_CH.EXE movie which can be found in the \\MOVIES\CHEMSK folder.

We are going to draw the following two-chain DNA Strand:

1. On the General toolbar, in the Zoom box, set the zoom value back to 100%.
2. On the Drawing toolbar, click **Polyline** .
3. Drag vertically down from the starting point of the curve to extend the direction line.
4. Release the mouse button.
5. Move the mouse to the right and down (as shown in the scheme below) to draw the curve.
6. Drag vertically down to extend the direction lines.

> **Tip** By changing the length of the direction lines you can modify the form of the curve.

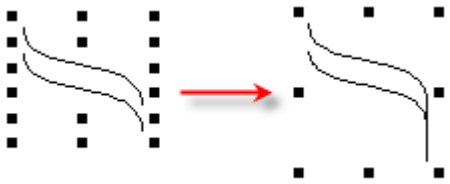
7. Release the mouse button, and right-click twice to finish drawing the curve and to activate the **Select/Move/Resize** tool:



8. Point to the selected curve and, while holding down CTRL+SHIFT, drag it down.

> **Note** 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 either by dragging the selection rectangle around them or by clicking each of the curves while holding down SHIFT, and then, from the **Object** menu, choose **Connect Lines** to connect the right ends of the curves:

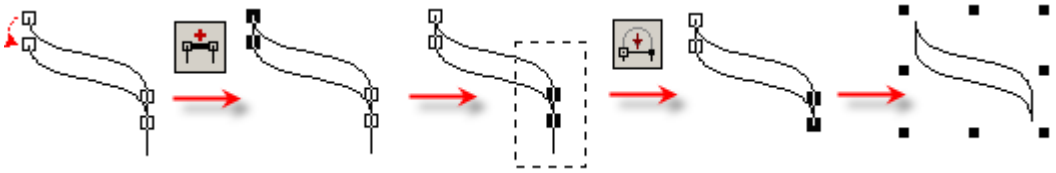


10. On the Editing toolbar, click **Edit Nodes**  , and proceed with the following to draw a segment:

    a. On the Node toolbar, click **Connect Vertices**  to connect the left terminal nodes with a line.

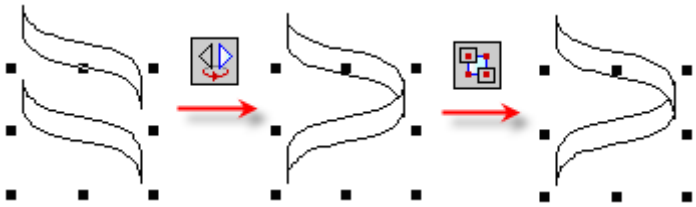
    b. Select the two right nodes by dragging the selection rectangle around them, and then, on the Node toolbar, click **Convert to Line**  .

    c. Right-click to leave the Edit Nodes mode and to switch to the **Select/Move/Resize** tool  :



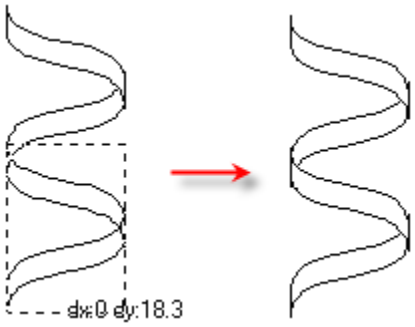
11. Make a copy of the obtained segment by dragging it with CTRL+SHIFT as described above in step 8.

12. 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.

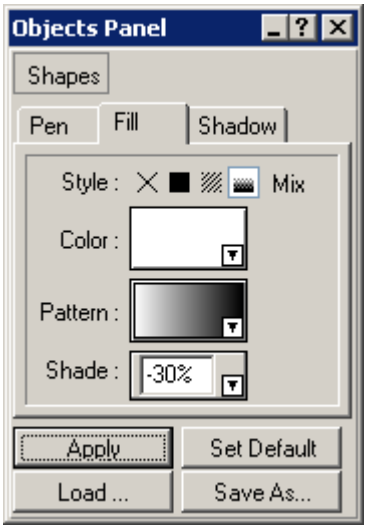


> **Tip** It may take some time to correctly position the segments by manually moving them. To align their position automatically, select both the segments, and apply the **Center Horizontally** tool  to the segments.

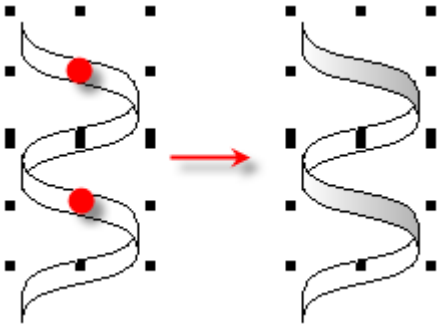
13. Select both the segments either by dragging the selection rectangle around them or by clicking while holding down SHIFT, and make a copy (holding down CTRL+SHIFT while dragging). Correct the position if necessary:



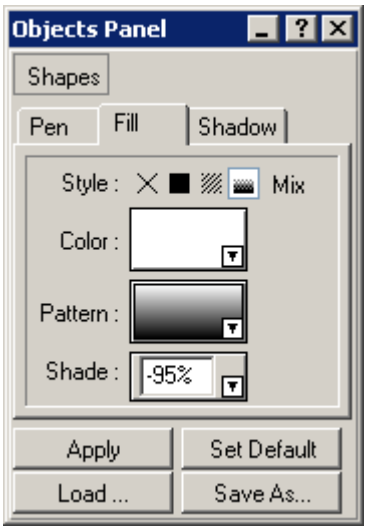
14. Select the segments marked with bullets in the scheme below by clicking them while holding down SHIFT.
15. Double-click any of the segments to open the **Objects** panel:



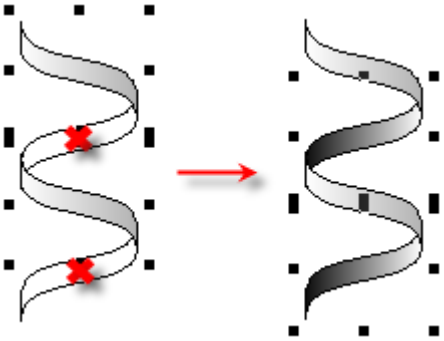
16. On the **Fill** tab, specify the above settings, and then click **Apply**:



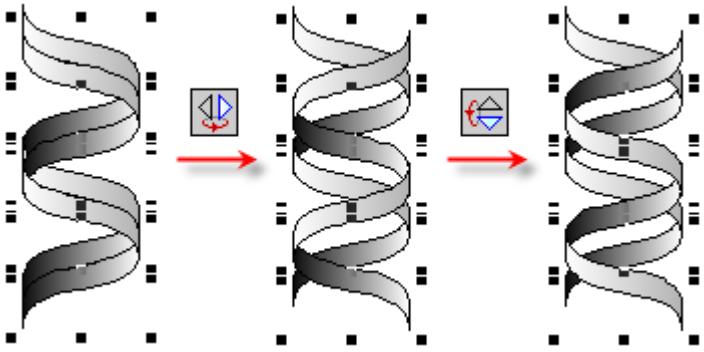
17. Select the other two segments (marked with crosses in the scheme below), and specify the following settings on the **Objects** panel:



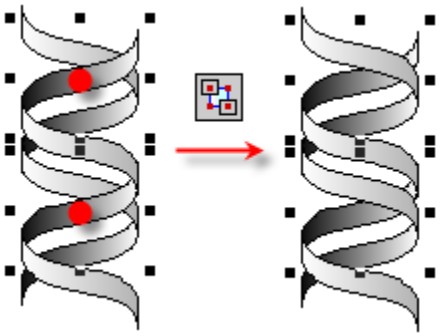
18. Click **Apply** to obtain the following spiral picture:



19. Close the **Object Panel** dialog box.
20. 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+SHIFT.
21. On the Editing toolbar. click **Flip Left to Right**  , and then click **Flip Top to Bottom**  :



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



23. Select all of the segments, and group them.

> **Note** The CHAPTER9.SK2 file (Page 4/6) with the two-chain DNA strand can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

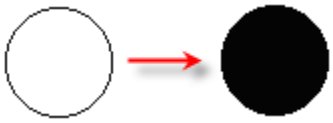
24. On the General toolbar, click **New Page**  .

9.6 Drawing Lipids and Micelles

This section explains how to create the pictures of lipid and micelle.

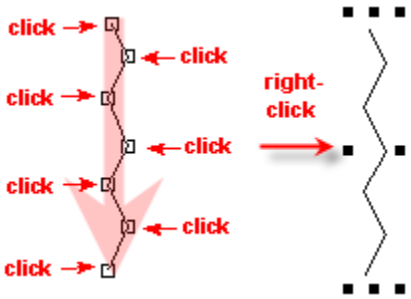
9.6.1 Drawing a Lipid

1. On the Drawing toolbar, click **Ellipse**  .
2. Drag in the workspace while holding down SHIFT to draw a circle.
3. Click the black color of the Color palette to fill the circle—this will be a phospholipid body:



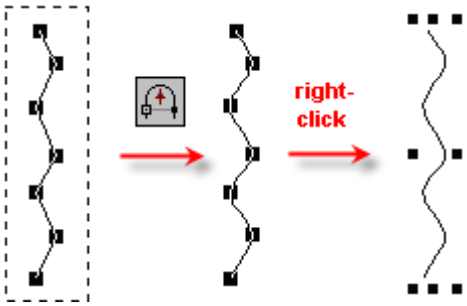
4. On the Drawing toolbar, click **Polyline**  .

5. Click repeatedly in the workspace to draw the carbonic tail, and then 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.

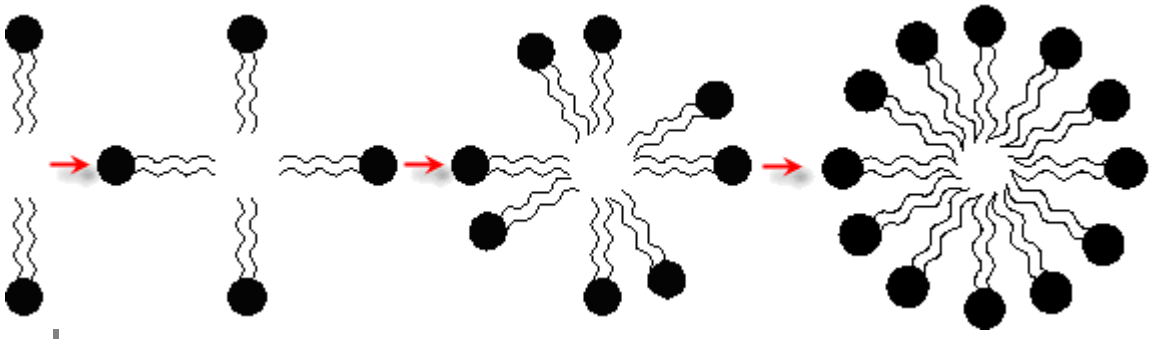
6. With the zigzag line selected, click **Edit Nodes** and smooth the line in the following way:
   a. Select all the nodes of the drawn line by dragging the selection rectangle around it. Note that selected nodes become black.
   b. On the Node toolbar, click **Convert to Curve**, and then click **Smooth**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



7. Point to the curve and drag it right while holding down CTRL+SHIFT to leave the copy of the curve behind.
8. Select both of the curves, and then arrange them as tails as shown at the beginning of the section by dragging them to the phospholipid body.
9. Select, and then group elements of the phospholipid by clicking **Group** on the Editing toolbar.

9.6.2 Drawing a Micelle

Following the general scheme given below, draw the phospholipid micelle using the copying feature (hold down CTRL+SHIFT while dragging), **Group**  , **Rotate 90°**  , and **Select/Move/Rotate**  tools, as well as the aligning and flipping tools:

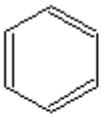
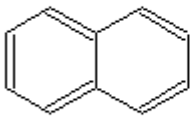
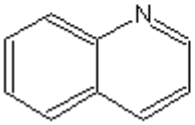


Note The CHAPTER9.SK2 file (Page 5/6) with the micelle can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
To switch to the required page, use the corresponding buttons on the Status bar.

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 the table.

As an example we will draw the following table:

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

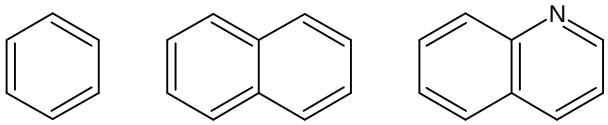
9.7.1 Drawing Table Contents

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

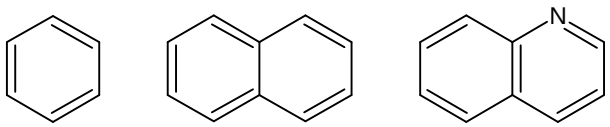
1. On the General toolbar, click **New Page**  .
2. Switch to the Structure mode.

3. Draw the structures of benzene, naphthalene, and quinoline using the technique described in the previous sections:

   Tip You can also find these structures using the **Dictionary** tool of the References toolbar.



4. Switch to the Draw mode, on the Drawing toolbar, click the white triangle on the **Text** button, choose the **Artistic Text** tool from the drop-down panel that appears, and then input the names for each of the structures:



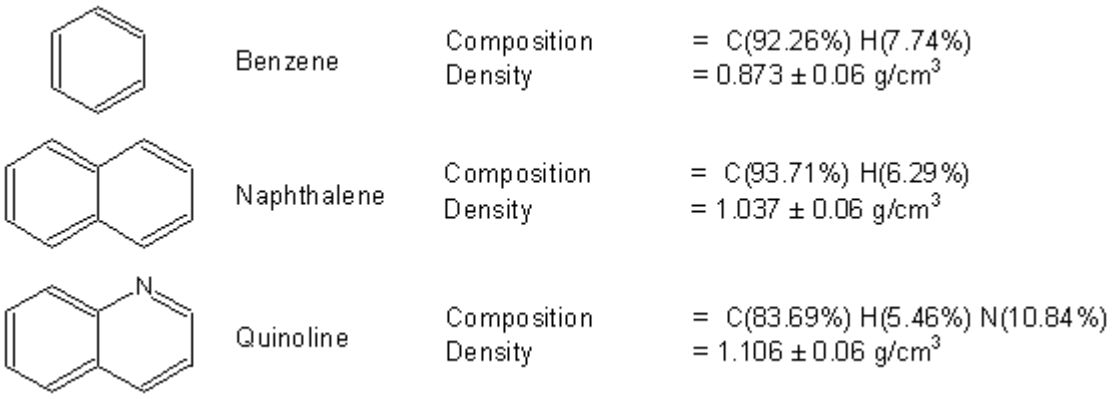
Benzene Naphthalene Quinoline

   Tip You can also name these structures using the **Generate Name for Structure** button on the General toolbar.

10. Now, return to the Structure mode, and calculate the Composition and Density properties for each of the compounds in the following way:
    a. On the **Tools** menu, point to **Calculate**, and then choose **Select Properties to Calculate**.
    b. In the **Select Properties to Calculate** dialog box that appears, click **Unselect All** Unselect All.
    c. On the **Properties** list, select ***Composition*** and ***Density***, and the click **OK**.
    d. Select the structure whose properties are to be calculated.
    e. On the **Tools** menu, point to **Calculate**, and then choose **Selected Properties**.
    f. In the **Calculation Results** dialog box that appears, click **Copy To Editor** Copy To Editor to paste the results as text to the workspace, and then move the text to an appropriate position.
    g. Switch back to the Structure mode.
    h. Repeat steps d–g for the rest of the structures.

    Note For more details on how to calculate properties individually, refer to Chapter 6.

5. Switch back to the Draw mode, and arrange the structures and text in the workspace for better viewing. You should obtain something like the following:



6. Choose the **Artistic Text** tool, click the empty space, and type *Structure*. Then click outside the text box.
7. In the similar way input *Name* and *Properties*. These are going to be the table headings:

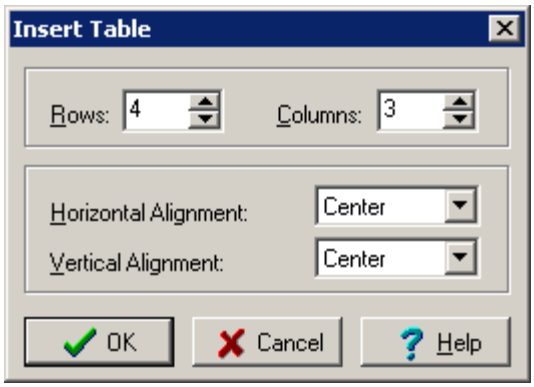
Structure Name Properties

> **Note** The current bold blue style of the caption text has been previously set in Section 9.4.1.1. You will change it later, in Section 9.7.4.

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.
2. In the **Insert Table** dialog box that appears as you release the mouse button, set the number of rows and columns to 4 and 3 correspondingly:

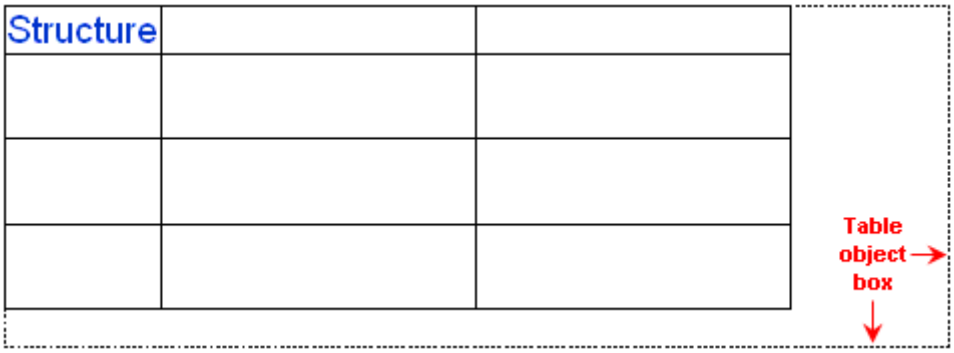


3. Click **OK**. The empty table is inserted.
4. Right-click to leave the Table drawing mode.

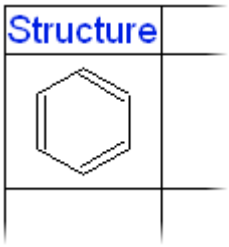
9.7.3 Placing Data into Table

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*** text 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):

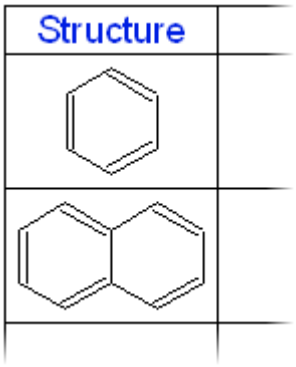


2. Now drag the benzene structure to the cell right below the Structure heading. Note that the cell size changes correspondingly:

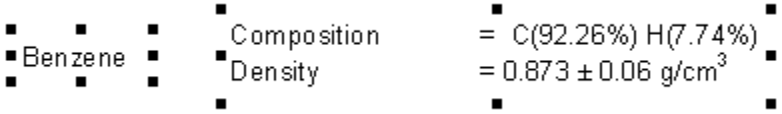


> **Tip** If the last row of the table is not fully visible after the above operation, click the table to select it, and then drag down the lower anchor point of the Table object box.

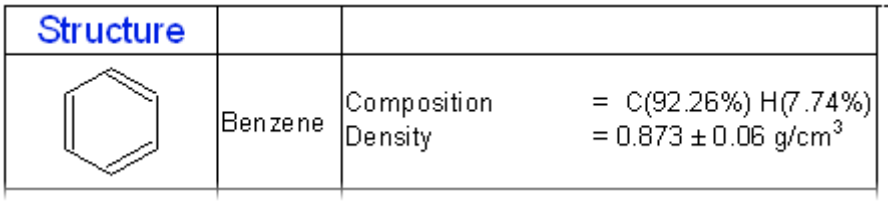
3. Another way of filling in the table cell is as follows: click the naphthalene structure to select it, hold down SHIFT and click an empty cell below the cell with the benzene to select both objects. On the Editing toolbar, click **Group**  The structure is automatically placed into the cell and the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



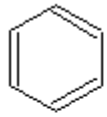
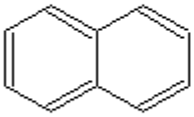
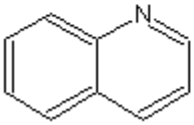
4. You can also add several objects to table at once: click the ***Benzene*** text, then hold down SHIFT and click the properties related to benzene to select both the objects.



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:



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

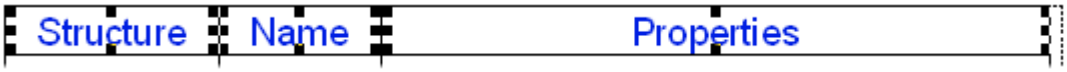
Structure	Name	Properties
	Benzene	Composition = C(92.26%) H(7.74%) Density = 0.873 ± 0.06 g/cm^3
	Naphthalene	Composition = C(93.71%) H(6.29%) Density = 1.037 ± 0.06 g/cm^3
	Quinoline	Composition = C(83.69%) H(5.46%) N(10.84%) Density = 1.106 ± 0.06 g/cm^3

Tip If the text or any of the graphics are not fully visible, click the table to select it, and then drag the corresponding anchor point of the Table object box.

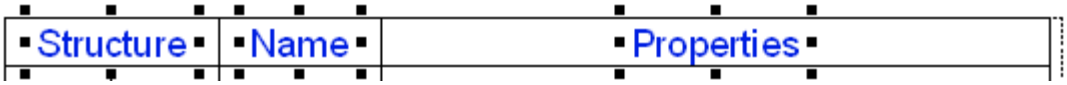
9.7.4 Modifying Table Contents

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

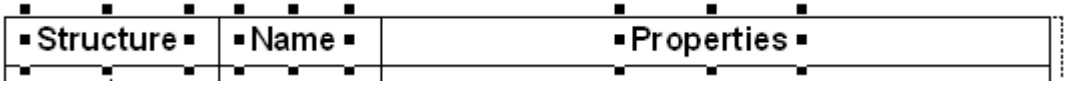
1. Ensure that the **Select/Move/Resize** tool is active, and drag over the upper row of cells to select them:



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:



3. Double-click any of the text elements to display the **Objects Panel** dialog box.
4. On the **Font** tab, select the **Bold** check box, set the font size to 12 and color to black, and then click **Apply**:



5. Close the dialog box.
6. Click somewhere in the empty space to cancel selection of the elements.
7. To place the text back into the table cell, select the text, hold down SHIFT, and select the cell where the selected text should be placed:

8. Click **Group**. The cell and contents are now grouped in a single object—you can see that when selecting the cell:

9. Another way of grouping is to point to the text and drag it a little within the borders of the cell. As you release the button, the text will be automatically grouped with the cell.

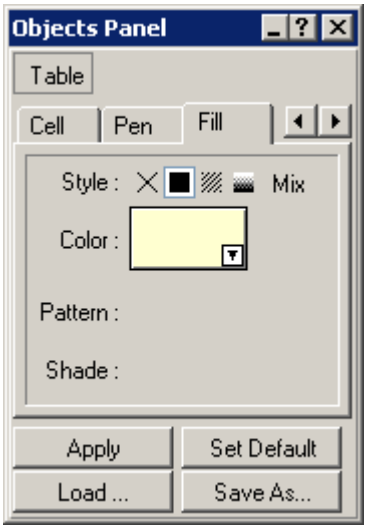
> **Tip** To understand whether the object and the corresponding cell are grouped, point to the object: if the whole cell is surrounded with the selection frame, not the object only, the object has been inserted into the cell.

10. Using any of the methods described, place all of the headings into the corresponding cells.
11. Select all of the data cells of the **Properties** column, and double-click the selection to open the **Objects Panel** dialog box.
12. Switch to the **Cell** tab, and then, in the **Horizontal** box, select ***Left*** to arrange the data along the left side of the column.
13. Click **Apply**, and then close the dialog box.

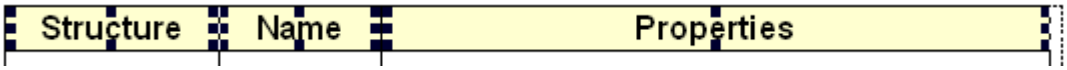
9.7.5 Editing Table View

Finally, we can modify the table view:

1. Ensure 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** dialog box.
3. Click the right arrow to display the **Fill** tab and then switch to the tab.
4. Set the fill color to ivory:



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



6. Close the dialog box.
7. Select the entire table, and double-click it to display the **Objects Panel** dialog box (note that the color is set to mixed on the **Fill** tab).
8. Switch to the **Pen** tab, change the color to crimson, and click **Apply**.
9. Close the dialog box.
10. Click somewhere in the empty space to cancel selection of the table elements and view the results.
11. Close the dialog box, save the file, and then close the document.

> **Note** The CHAPTER9.SK2 file (Page 6/6) with this table can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.
> To switch to the required page, use the corresponding buttons on the Status bar.

10. Managing Documents

If you have worked over the material described in the previous chapters, you should have several ACD/ChemSketch documents 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; and
- Create a poster.

Sections within this chapter 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 of 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 **Header and Footer**, and then choose **Edit**. The header text box appears at the top of the page (to the left of the page's header), along with the floating Header and Footer toolbar:

2. Type the text to be a header o the page, for example, *ACD/ChemSketch*.
3. On the Headers and Footers toolbar, click **Go to Next Text**  .
4. In the text box that appears at the center of the page's header, type *Author:*.
5. On the Header and Footer toolbar, click **Insert AutoText**  , and choose ***Author***. Your login name template is automatically inserted.
6. Click **Go to Next Text**  again to insert one more text box to the right of the page's header.
7. Click **Insert AutoText**  , and choose ***Page X of Y*** to insert the corresponding text template.
8. If you want to add data to the page footer, click **Go to Next Text**  , and edit the footer in the aforementioned way.

> **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.

9. As soon as the required data is inserted, leave the Header and Footer Editing mode by clicking **Close** on the toolbar.
10. Switch between the pages to view the headers and footers inserted.

10.2 Converting to Adobe PDF

ACD/ChemSketch 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 convert your document to the Adobe PDF format.

> **Note** To be able to export file to PDF from ACD/ChemSketch, you do not have to install Adobe Acrobat or Adobe Reader on your computer, but to view PDF files, you should have any of them. You can install Adobe Reader when running ACD/ChemSketch setup program, or download Adobe Reader from http://www.adobe.com.

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** on the General toolbar to view the whole page.

2. On the General toolbar, click **Export to PDF**.
3. In the **Export** dialog box that appears, specify the name and location of your .PDF file, *e.g. Chapter10.pdf*, and click **Save**.
4. As soon as the conversion is completed, browse to the newly created file, and open it with Adobe Reader to view the results.

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

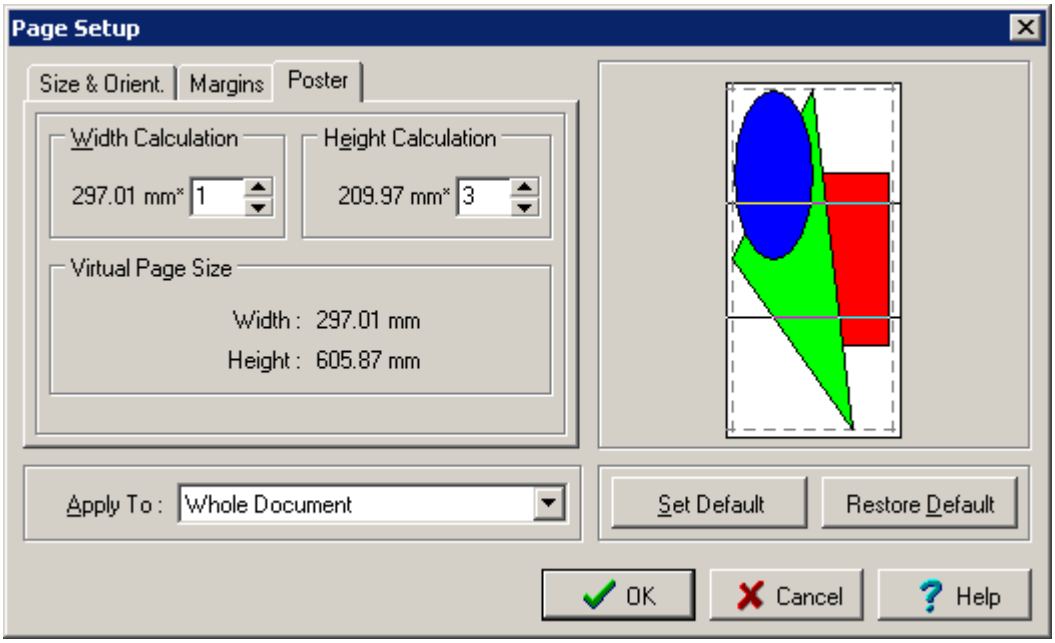
10.3 Creating a Multi-Page Poster

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 join them.

This section is based on the POSTER.EXE movie which can be found in the \\MOVIES\CHEMSK\ folder.

1. From the **File** menu, choose **Page Setup**.
2. On the **Size & Orient.** tab, set the size of an individual page (*i.e.*, the format of paper sheets used by your printer) and choose the **Landscape** option.
3. Switch to the **Margins** tab, and set the page margins.

4. Switch to the **Poster** tab. Set the number of standard pages you want your poster to consist of. You can see the automatically calculated size of the poster in the **Virtual Page Size** area:



5. Click **OK**.
6. Create your poster using the tools of the Structure and Draw modes.
7. Click **Full Page**  to see the general layout and arrange the poster elements as you prepare it.

> **Note** You can use the **Paste** and **Paste Special** commands from the **Edit** menu to insert objects (text, pictures, *etc.*) created in other Windows applications. You can also edit these objects using OLE. To do this, select the object choose **Edit <*Object Type*> Object** command from the **Edit** menu.

8. If you want to see how your poster will be divided into individual pages while being printed, from the **Options** menu, choose **Preferences**, and then, on the **General** tab of the **Preferences** dialog box that appears, under **Borders**, select the **Printable Area** check box.
9. From the **File** menu, choose **Print**. In the dialog box that appears, click **Print** to print your poster, and then join the pages.

> **Tip** You can also click **Print**  on the General toolbar.

11. Working with Styles in Structure Mode

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.

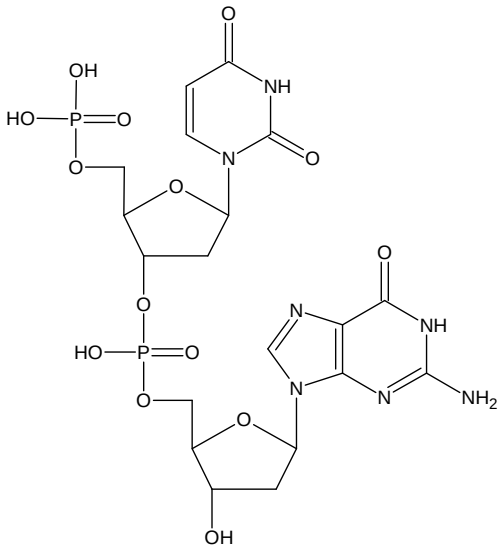
In this chapter, you will learn how to:

- Change the style of structures;
- Save your style;
- Apply an existing style; and
- 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 graphical objects and text) to which you can assign a name and save.

First of all, draw the following structure in the Structure mode of the program:



This structure can be drawn with the help of the **Template Window** dialog box (**DNA/RNA Kit** tab) from the 2-deoxyriboso-5-phosphate, uracil, and guanine components. For more details on how to draw structures using Template Window, refer to Section 5.5.

> **Note** The CHAPTER11.SK2 file with this structure can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.

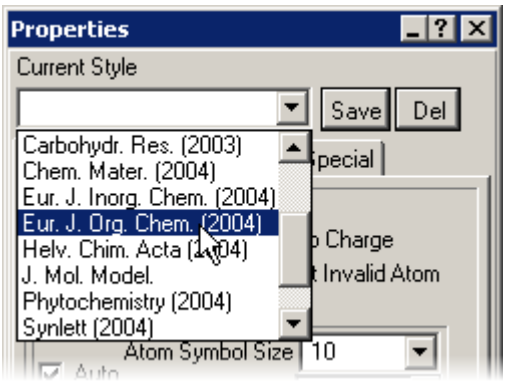
11.2.1 Applying a Journal Style

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

1. Select the structure using the **Select/Move** tool.

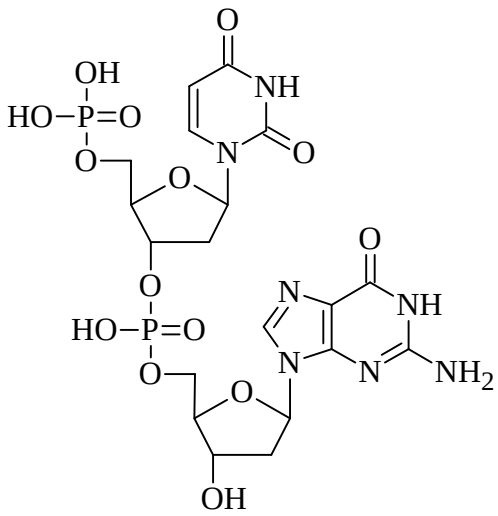
   > **Tip** You can also click near the structure for that.

2. Point to one of the selection squares on the structure so that they turn from "□" to "■", and double-click to display the **Properties** dialog box.
3. In the **Current Style** box, select ***Eur. J. Org Chem. (2004)***:



> **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. For more information on how to prepare the drawings for such publications, refer to the following section.

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



> **Note** The CHAPTER11.SK2 file with this structure can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.

5. From the **File** menu, choose **Save As** and save your structure to the DNAFRAG.SK2 file.
6. Select the whole structure again, in the **Properties** dialog box, from the **Current Style** list, select **Normal**, and click **Apply** Apply. The structure should appear as before.

   Tip You can also click **Undo** button on the General toolbar.
7. Close the dialog box.

11.2.2 Preparing for Publication

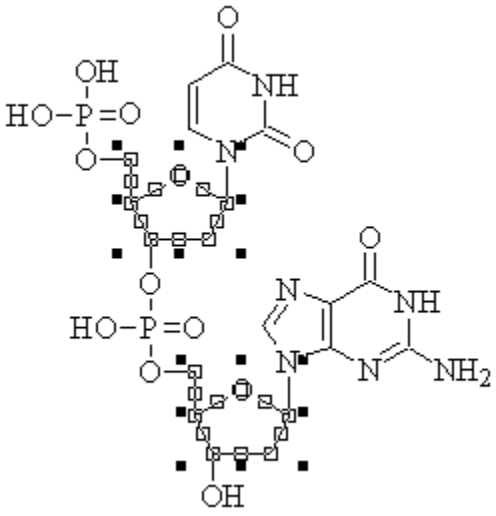
In addition to making your structural drawing conform to the guidelines of a particular journal, there are many other matters to arrange during manuscript preparation. For this reason, Advanced Chemistry Development has included **Instructions for Authors**, a hyperlinked list of guidelines for over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

1. From the **Help** menu, choose **Instructions for Authors**.
2. Find the ***Journal of Organic Chemistry*** in the list.
3. Click the link to the corresponding Web site or follow the indicated pathname of the Adobe PDF file to display the corresponding document with the *Guidelines for Authors*.
4. On the **Contents** tab of the Help window, expand the ***Instructions for Authors*** heading to view to the list of available journals so you can view their guidelines too.

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 and ensure that you are in the Structure mode.
2. Switch to the **Lasso On** tool and click **Select/Move**.
3. Select the sugar components while holding down SHIFT:

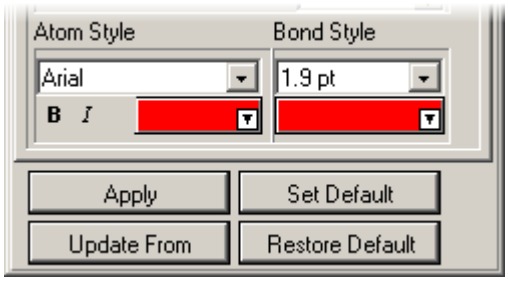


4. Point to any part of the selected fragment so that the selection squares become black, and double-click to display the **Properties** dialog box.

11.3.1 User-Defined Style: Sugar

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

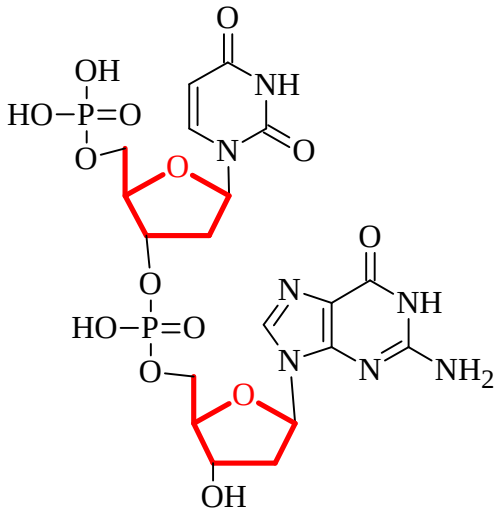
1. In the **Atom Style** and **Bond Style** areas, specify the color for the selected fragments (for example, red) and set the bond width to a different value (for example, *1.9 pt*):



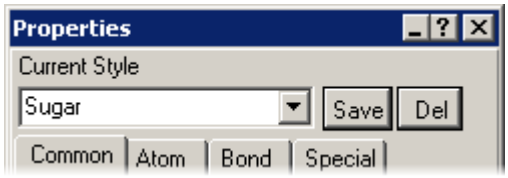
> **Note** Units of measurement used in most of the panels within ACD/ChemSketch correspond to those set in the **Preferences** dialog box (**Options** menu). You may set values for width, length, *etc.* in points/inches/millimeters/centimeters. Type the values and add the unit you want (pt/in/mm/cm),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

2. Click **Apply** 

and click outside the structure to cancel the selection. As you can see, the selected segments are now colored with red:



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

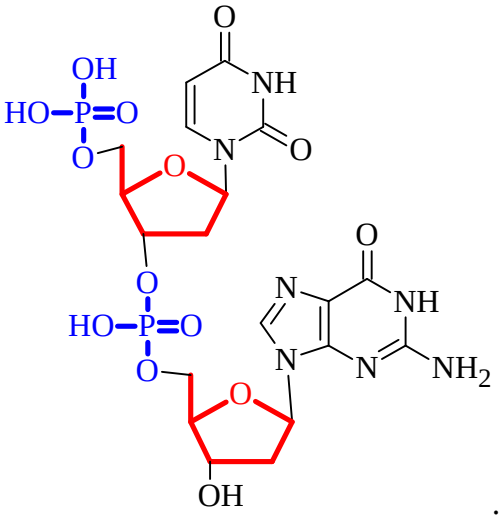


4. In the **Save Style** panel that appears, click **Yes**.

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 parts of the structure, and define the same thick bond width and blue color for the bonds and atom fonts.
2. Save this style as *Phosphate*,
3. Click **Apply** Apply to apply the new style to the selected parts:

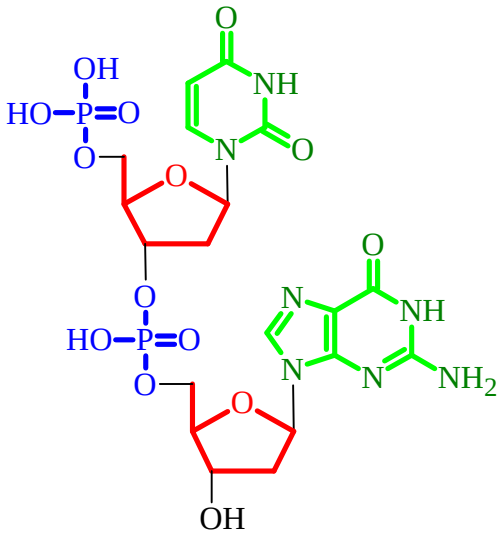


11.3.3 User-Defined Style: Base

We can also define our own style for the bases:

1. Select the base parts of the structure, and set the color of the atom symbols to dark green, the bonds to neon green, and define the same thick bond width.
2. Save this style as *Base.*
3. Click **Apply** Apply to apply the new style to the selected parts.

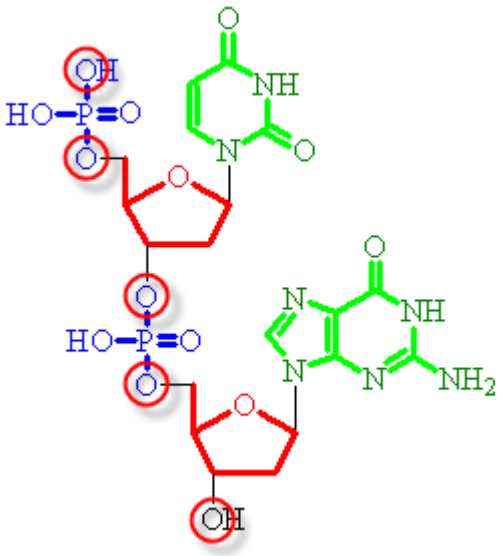
4. Arrange all of the fragments that were shifted when changing their style. The structure now should look like this:



11.3.4 User-Defined Style: Highlight

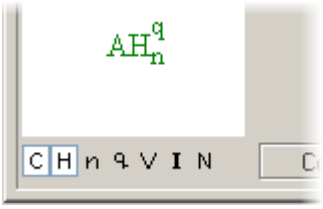
Perhaps, during the course of your presentation you want to draw the attention of the audience to the oxygen atoms. We will create a fourth style, *Highlight*, for this:

1. Holding down SHIFT, click the oxygen atoms indicated below to select them:



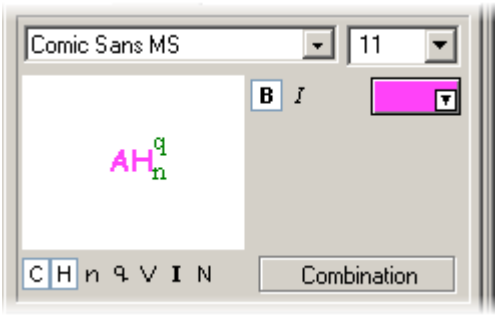
2. On the **Properties** dialog box, switch to the **Atom** tab.

3. Below the preview area, click the **C** and **H** buttons while holding down SHIFT to change the color and size of both the atom symbol (oxygen in this case) and hydrogen:



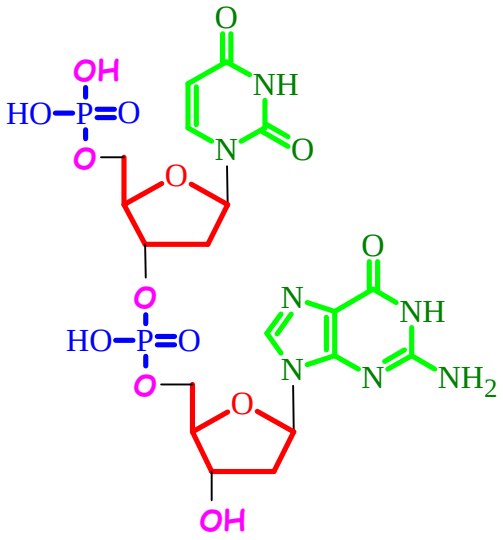
> **Note** You may also change other atom attributes (hydrogen index, charge, valence, isotope, numbering) by clicking the corresponding buttons.

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



> **Tip** You can also change the bond attributes in a similar manner.

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

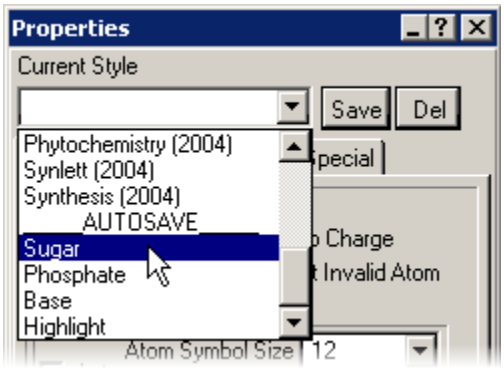


6. Save the style as *Highlight*.
7. Close the **Properties** dialog box.

11.4 Applying Existing Styles

To practice applying the styles you have just created, reopen the DNAFRAG.SK2 file.

1. Use the **Lasso** tool  to select the furanose rings as shown in Section 11.3.
2. From the **Tools** menu, choose **Structure Properties**.
3. On the **Properties** dialog box that appears, from the **Current Style** box, choose ***Sugar***:

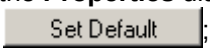


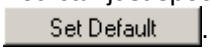
4. Click **Apply**  . The chosen style will be applied to the selected fragments.
5. Choose the phosphate groups.
6. From the **Current Style** box, choose ***Phosphate***, and then apply the style to the selected fragments.
7. Similarly, select the two bases in the DNA fragment, and apply the Base style to them.

> **Tip** The information about a user-defined style is stored on your local hard drive in the ACD/ChemSketch Private directory that is specified on the **General** tab of the **Preferences** dialog box, (to view the dialog box, on the **Options** menu, click **Preferences**), in a Style 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 file into their Private directory.

11.5 Setting a Default Style

You can specify the style to be applied to your structure drawings by default (*i.e.*, any structure drawn will be thereafter of that style) in one of the following ways:

- From the **Current Style** box of the **Properties** dialog box, choose the required style (e.g., ***Normal***), and click **Set Default**  ; or
- On the **Options** menu, point to **Set Structure Drawing Style**, and click the required style on the submenu to select it.

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

12. Working with Styles in Draw Mode

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, filled objects, arrows, and lines.

In this chapter, you will learn how to:

- Change an object's style;
- Save a style; and
- Set a default style.

12.2 Changing Style of an Object

In Chapter 9 there was a brief introduction to changing an object's style. In this section, we will acquaint you with 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** dialog box. Depending on the kind of selected object(s) (shape, linear object, arrow, text, spectrum, table, and/or structure), Objects Panel may contain different Object mode buttons (Common, Shapes, Text, *etc.*):

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

> **Note** Settings from the Common mode (click the **Common** Common button to turn this mode on) will be applied to all of the objects. For example, changing the pen color to red will affect shapes, lines, and structures. If you change any attribute in the Shapes Shapes mode, it will affect shapes only.

12.3 Saving Style

The style you have created can be saved:

1. To save the specified settings, on the **Objects Panel** dialog box, click **Save As** Save As....
2. In the **Save User Style** dialog box that appears, under **Include Object's Attributes**, 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. In the **Style Name** box, type the name for your style, and click **OK**. The style will be added to the list of styles. It can be then loaded to Objects Panel and applied to the selected objects or set as the default.

12.4 Applying 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** dialog box.
3. Click **Load** Load ..., and then, from the drop-down list of styles, choose the required one. The style attributes will be loaded into the panel.
4. Click **Apply** Apply.

12.5 Setting Default Style

The default style attributes can be specified on special Style panels that can be displayed using the corresponding 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** Load ... . The style is automatically loaded into other Style panels, where it is applicable, and becomes the default.

You can also load style attributes from the drawn object into any of the style panels:

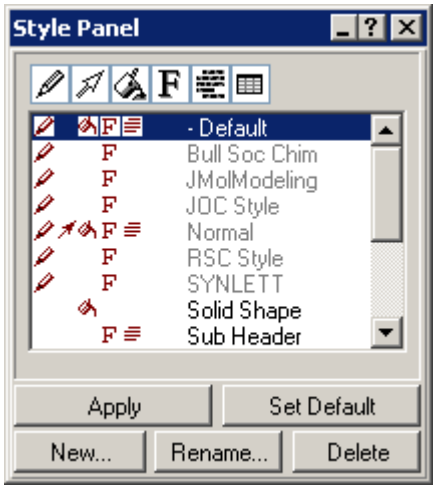
- Click **Update From** Update From (note that the mouse pointer changes to FROM), and then click the object. The object's style attributes are immediately loaded into every Style panel and are automatically set as the default.

> **Note** If you want to change the style of a specific drawn object without affecting the default one, use its own 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** dialog box:

- From the **Tools** menu, choose **Style Organizer Panel**.



In this dialog box, 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 **Apply** Apply .
Set the style as default	Select the needed style in the list, and click **Set Default** Set Default .
Create a new style based on the current default settings	Click **New** New... .
Rename the style	Select the needed style in the list, and click **Rename** Rename... . 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 **Delete**  . Note that the built-in styles (appearing in gray in the list) cannot be deleted.

13. Creating Report Templates

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, Calc 2D NMR, MASS, UVIR, Curve, and Chrom modules of ACD/SpecManager, ChemFolder, ChromGenius, PhysChemHistory, PhysChemDatabase, AutoChrom. Later, we are going to enlarge the list of programs which allow the creation of template-based reports. With the Report Template tool, it is easy to meet your corporate standards.

Using ACD/Report Template, you can, for example, arrange various 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; and
- Save the template to a separate file; and
- Use the created templates.

> **Note** Prior to performing any of the procedures described below, ensure that you are in the Draw mode of ACD/ChemSketch.

13.2 About Report Templates

Each report template has its inherent set of ***template objects*** (or just ***objects***) that can be common (text label, formatted text) or assigned to certain ACD/Labs program (*e.g.*, spectrum, table, graph, chemical structure). Each object has concrete set of properties which regulate its appearance. For the most part, these properties are correlated with properties in the corresponding program. If template objects have different identification numbers (***ID***), they refer to different ACD/SpecManager documents. If there are no IDs assigned, all objects in this template refer to the same ACD/SpecManager document.

It is possible to insert your company logo into template-based reports as a bitmap (for more information on how to insert a bitmap, refer to the corresponding topic in the *Report Template Help* located in the ACD/Labs installation directory, \\REPTEMPL.CHM).

Moreover, as soon as the template-based report is ready, you can easily insert all proper corrections using **ACD/ChemSketch Objects** panel which appears immediately by double-clicking.

13.3 Creating Template Objects

There is 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.

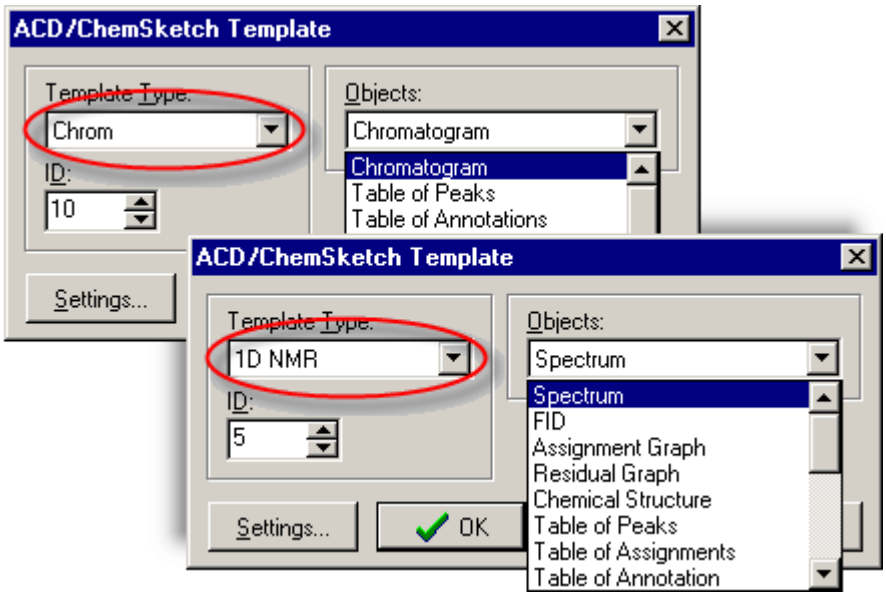
13.3.1 Inserting Spectrum Objects

1. Switch to the Draw mode.
2. On the Drawing toolbar, click **Report Template**  . Note that the information cursor  appears.
3. With the Report Template mode on, point to the top left corner of the workspace, 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 later.

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

> **Note** Depending on the module's name chosen from the **Template Type** list, the adjacent **Objects** list looks different:



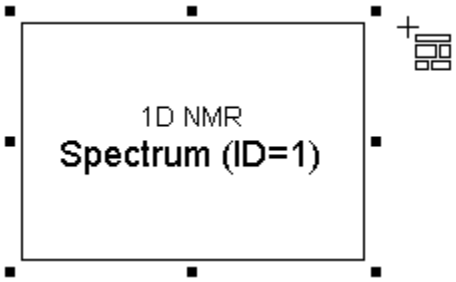
When you choose a different template type in the list, the caption of the template object in the ChemSketch workspace changes correspondingly.

We are going to create a template for 1DNMR and 2DNMR modules (however, if you do not have these modules of ACD/SpecManager, select other template types instead):.

5. In the **Template Type** list, select ***1D NMR***, and then, in the **Objects** list, select ***Spectrum***. Note that the object's caption in the workspace changes to ***1D NMR Spectrum***.
6. In the **ID** box, enter *1* to refer this object to a spectral document with the same ID. Note that the object's caption in the workspace becomes ***1D NMR Spectrum (ID=1)***.

Note For more information on how to assign IDs to ACD/SpecManager documents, refer to the corresponding *How to create a template-based report* topic of the *Report Template Help* located in the ACD/Labs installation directory, \\REPTEMPL.CHM. This Help is also a constituent of both ACD/ChemSketch Help and ACD/SpecManager Help.

7. Click **OK** to close the **ACD/ChemSketch Template** dialog box. Note that the Report Template mode is still active:



8. Drag in the workspace to the right of the first object to draw a second template object approximately of the same size.
9. In the **Template Type** list of the **ACD/ChemSketch Template** dialog box that appears, select ***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:

10. In the **ID** box, enter *2*. Keep the dialog box opened.

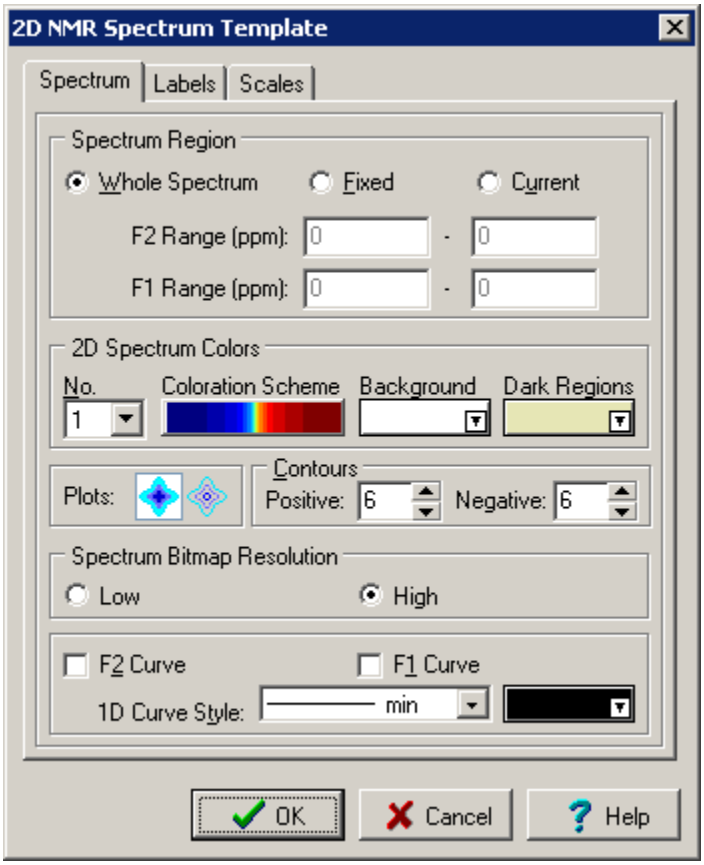
Tip If you have only a single module of ACD/SpecManager on your PC, and therefore, only a single module name is available from the **Template Type** list of the **ACD/ChemSketch Template** dialog box, insert two instances of spectrum / chromatogram / curve (later on, spectrum) of the same type but assign different IDs to them. When creating a report according to this template, you will be able to insert two different spectra, chromatograms, or curves.

13.3.2 Setting Display Preferences

As the 2D spectrum object is created, you can set the display preferences for it at once:

1. Click **Settings** 

to display the **2D NMR Spectrum Template** dialog box where you can set the display preferences for the 2D spectrum objects:



> **Note** Each template object has its inherent set of options included into a corresponding dialog box. For more information on the options available in the dialog box for a given object, click **Help**.

We are going to set the display preferences which are common for the majority of ACD/SpecManager modules:

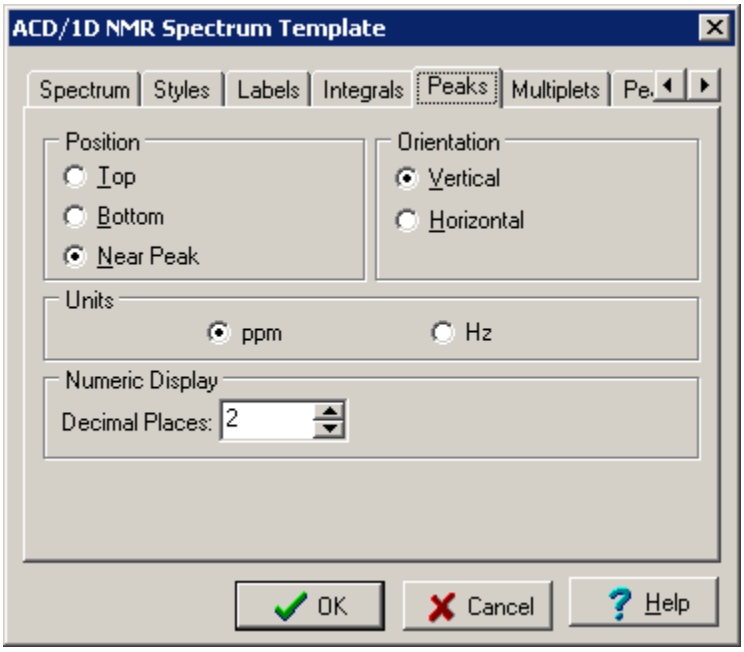
2. In the **Spectrum Region** area of the **Spectrum** tab, click **Whole Spectrum**. In this case, the entire spectrum will be inserted into reports made according to this template.

> **Note** If you select **Fixed** or **Current**, only a specified region will be inserted.

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

Now, let's customize display preferences for the previously created template object of the 1D NMR spectrum:

1. Double-click the 1D NMR spectrum object to make it active and to display the **ACD/ChemSketch Template** dialog box.
2. Ensure that the ***Spectrum*** item is selected in the **Objects** list, and click **Settings** Settings....
3. In the **ACD/1DNMR Spectrum Template** dialog box that appears, click the **Peaks** tab:

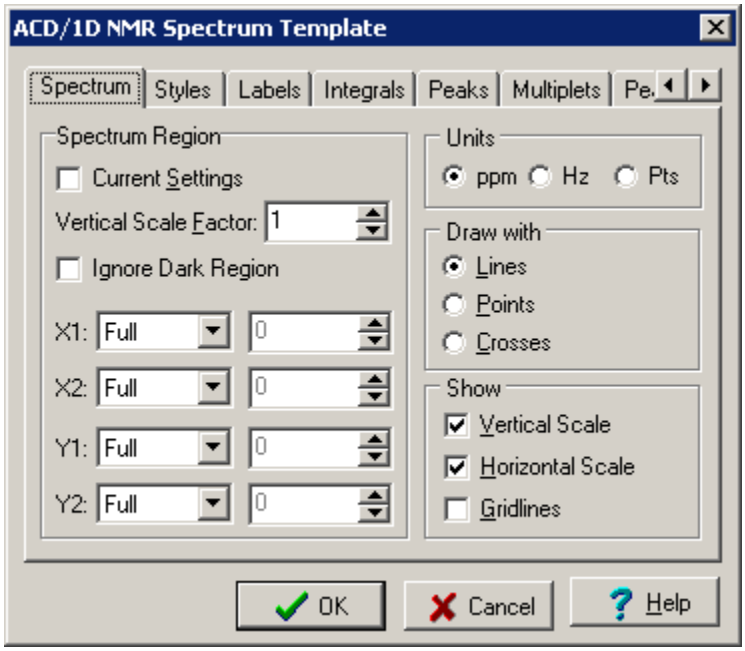


4. Specify the display of the peak labels: in the **Position** area, click **Near Peak**, and, under **Orientation**, click **Vertical**.
5. In the **Numeric Display** area, enter *2*. In this case, two decimal places will be displayed in peak labels.

> **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, *etc*.).

6. Switch to the **Spectrum** tab.

7. In the **Spectrum Region** area, ensure that the **X1**, **X2**, **Y1**, and **Y2** options are set to ***Full***, and, in the **Show** area, select the **Vertical Scale** and **Horizontal Scale** check boxes:



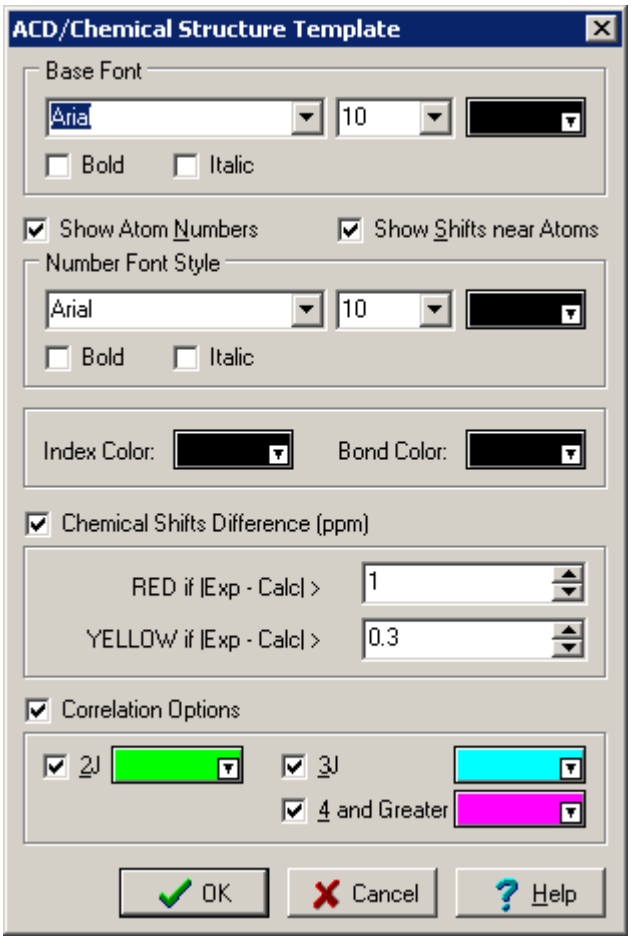
> **Note** Although you do not see any immediate outcome when setting display preferences, the settings are stored by the program and placed into the corresponding template object.

8. Look through the other tabs in your module-related dialog box to find out what other options are available, set other options if required (for more information on the options available, click **Help**), and then click **OK** to apply the changes.
9. In the **ACD/ChemSketch Template** dialog box, click **OK** to close it.

13.3.3 Inserting Structure and Spectrum Parameters Objects

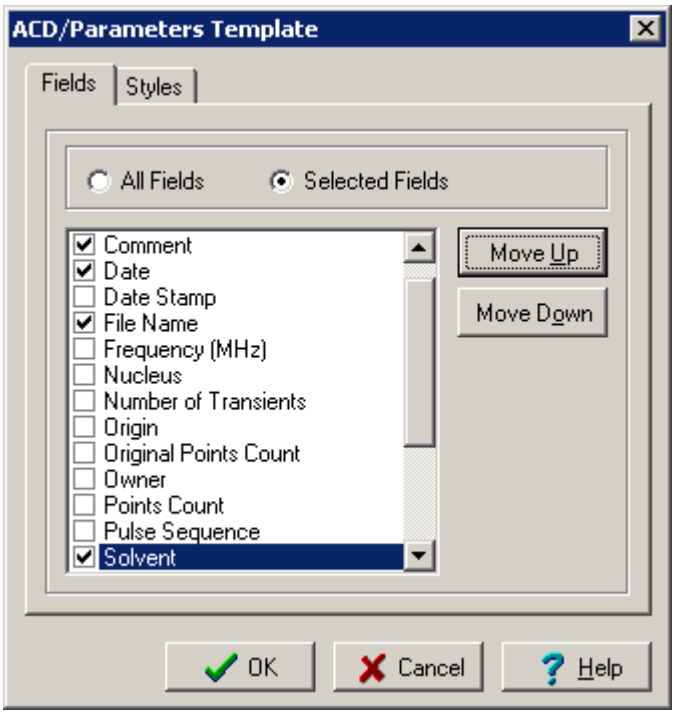
1. Select the **Report Template** tool again, and insert a ***Chemical Structure*** object of the 1D NMR template type with ID=1 (using the drawing instructions of Section 13.3.1).

2. In the **ACD/ChemSketch Template** dialog box, click **Settings** Settings... to customize the display of the structure:



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

9. On the **Fields** tab of the **ACD/Parameters Template** dialog box that appears, choose the **Select Fields** option 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.
10. Right-click in the list of parameters, and, from the shortcut menu that appears, choose **Unselect All** to clear all check boxes, and then select ***Comment***, ***Date***, ***File Name***, and ***Solvent***. The selected fields will be inserted into the report:



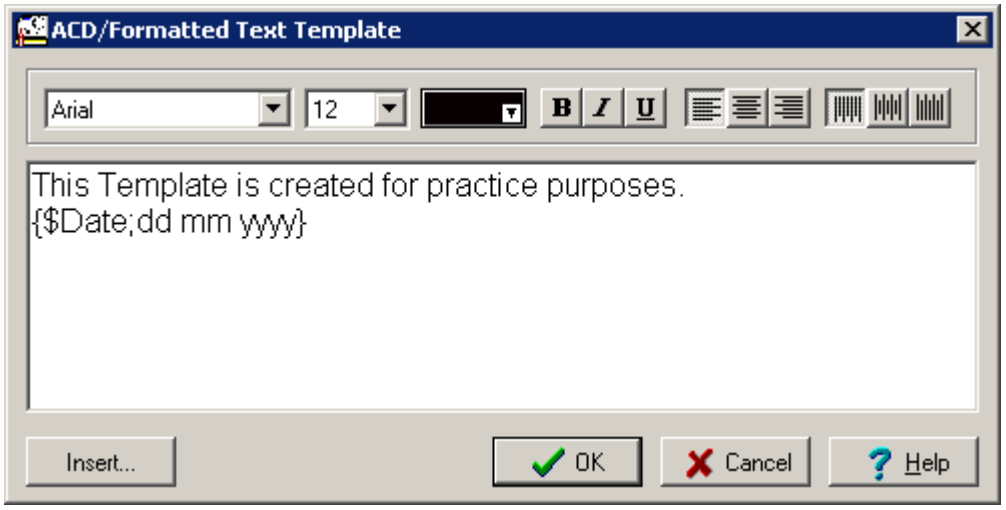
> **Note** You can use the **Move Up** Move Up and **Move Down** Move Down buttons to rearrange the fields order in the list.

11. Switch to the **Styles** tab.
12. Select the **Show Borders** check box to show horizontal and vertical borders between each Name-Value pair.
13. Select the **Show Names** check box to show the field names, otherwise only the values will be displayed.
14. Select the **One Column** check box to show parameters in a column: one Name-Value pair under another.
15. Click **OK** in both the dialog boxes.

13.3.4 Subscribing Template

Now we are going to add a subscription to the template.

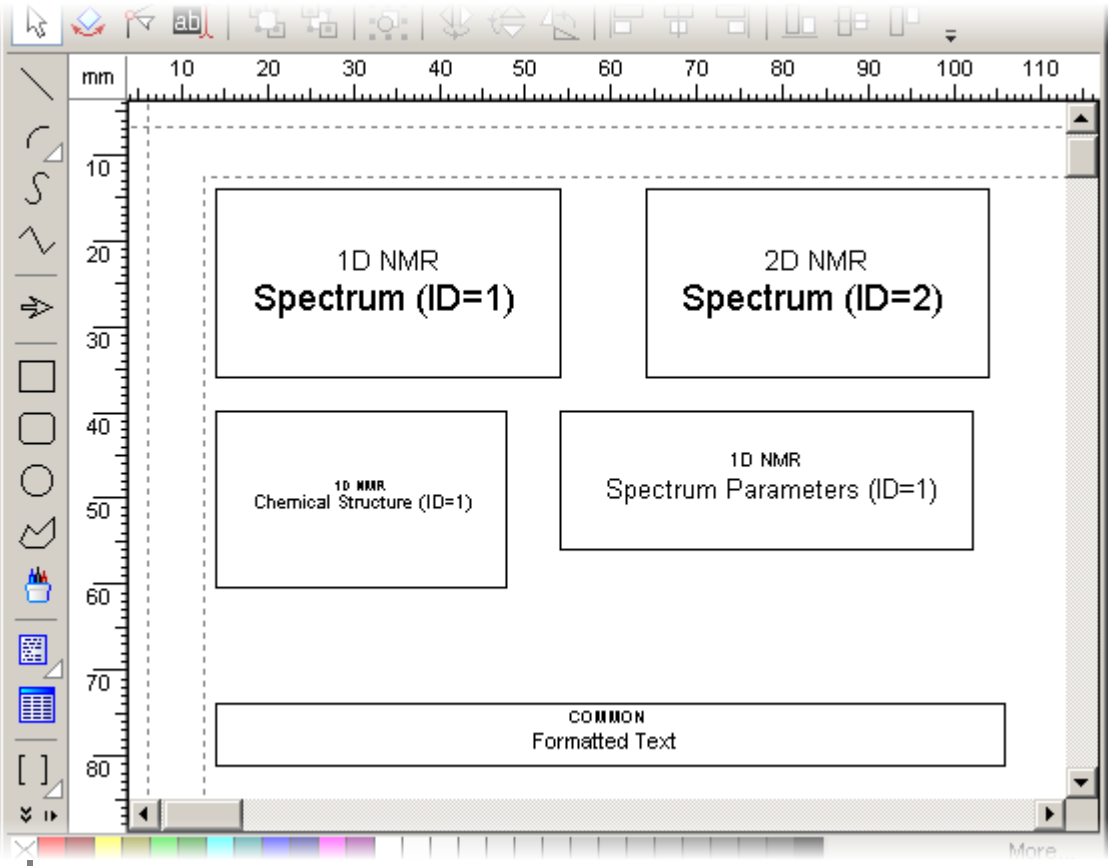
1. Make sure that the **Report Template** tool is on, and insert a long narrow box along the bottom border of the template page using the drawing instructions listed above.
2. In the **ACD/ChemSketch Template** dialog box that appears, select ***COMMON*** in the **Template Type** list, and then, in the **Objects** list, select ***Formatted Text***.
3. Click **Settings** Settings... to display the **ACD/Formatted Text Template** dialog box. Using this dialog box, you can add any textual information to the template which will appear in any report made according to this template.
4. In the text box, type a few words in the first text line 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*.
5. Press ENTER to start the next text line.
6. Click the **Insert** Insert... button to display the **Select Field** dialog box where you can specify the current date, time, or page number to be automatically inserted in the template page.
7. In the **Name** list, select ***$Date***, and then click **OK**.
8. Select the text, and set the font and alignment preferences for it as desired using the tools available at the top of the dialog box:



Note The Alignment buttons located in the upper right corner of the 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's border.

9. Click **OK** in both the dialog boxes.

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



Note The CHAPTER13.SK2 file with this template can be found in the ACD/Labs example folder, \\ACD\EXAMPLES\CHEMSK\.

13.4 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 by clicking it.
3. Using the following instructions, resize and rearrange the template objects to suit your requirements:
   a. Point to the inside of the template object making notice that the mouse pointer changes to . Now, you can relocate the object by dragging it.
   b. Point to any node of the selected object box making notice that the mouse pointer changes to a double-headed arrow of the corresponding direction. Now, you can resize the object by dragging it.

Tip From the **Options** menu, choose select **Snap on Grid** and/or **Show Grid** to make your object-arranging work easier.

13.5 Saving 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:

- From the **File** menu, choose **Save As** to display the **Save Document As** dialog box, and then specify the name and location for the ACD/ChemSketch file.

13.6 Applying Templates

As soon as ACD/ChemSketch is an integrated part of the most ACD/Labs software, you can immediately apply a template created within the ChemSketch window of an ACD/Labs application to report the desired data.

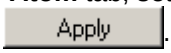
In the following example, we will assume that ACD/SpecManager package with ACD/NMR WorkBook is installed and started on your computer, and the template-based report is created:

1. Switch to the Processor window.
2. From the **View** menu, choose **ACD/NMR WorkBook** to display the corresponding panel (if it is not displayed yet).
3. On the toolbar of the empty ACD/NMR WorkBook panel, click **Start Working With Project** 

. From now on, the toolbar contains two buttons allowing you either to create a new project or open an existing one.

   Note This step is required only when launching ACD/NMR WorkBook for the first time.
4. Click **Open**  .
5. In the **Open Project** dialog box that appears, specify the ACD/SpecManager Project file located in the ACD/Labs example folder, \\EXAMPLES\SPECMAN\2DNMR\NMR_PROJ\STRYCH-TEST.SMP.
6. Click **Open** to load the project to the Processor window.
7. From the **Edit** menu, point to **Create Report**, and choose **by Template**.
8. In the **Select Report Template** dialog box that appears, select the location and file name of the ACD/ChemSketch template you have previously created.
9. Click **OK**.
10. After the report is created, you are automatically transferred to the ChemSketch window.

If necessary, you can further edit the report objects that are not correctly displayed:

1. Go to the first page of the report, and double-click the Structure object to display the **Objects Panel**.
2. On the **Atom** tab, set the symbol size to *10* and color to navy blue, and then click **Apply** 

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