

ACD/Structure Drawing Applet (SDA)

Version 8.0 for Microsoft Windows

Tutorial

Drawing Structures with SDA

Advanced Chemistry Development, Inc.

Copyright © 1996–2004 Advanced Chemistry Development, Inc. All rights reserved.

ACD/Labs is a trademark of Advanced Chemistry Development, Inc.

Microsoft and Windows are registered trademarks of Microsoft Corporation in the United States and/or other countries Copyright © 2004 Microsoft Corporation. All rights reserved.

IBM is a registered trademark of International Business Machines Corporation Copyright © IBM Corporation 1994, 2004. All rights reserved.

Adobe, Acrobat, PDF, Portable Document Formats, and associated data structures and operators are either registered trademarks or trademarks of Adobe Systems Incorporated in the United States and/or other countries Copyright © 2004 Adobe Systems Incorporated. All rights reserved.

Camtasia is a registered trademark of TechSmith Corporation, and Camtasia Studio is a trademark of TechSmith Corporation Copyright © 1999-2004 TechSmith Corporation. All rights reserved.

CambridgeSoft and ChemDraw are registered trademarks of CambridgeSoft Corporation Copyright © 2004 CambridgeSoft Corporation. All rights reserved.

Java is a trademark or registered trademark of Sun Microsystems, Inc. in the U.S. or other countries Copyright © 2001–2004 Sun Microsystems, Inc. All rights reserved.

All the other trademarks mentioned within this tutorial are the property of their respective owners.

All trademarks are acknowledged.

Information in this document is subject to change without notice and is provided “as is” with no warranty. Advanced Chemistry Development, Inc., makes no warranty of any kind with regard to this material, including, but not limited to, the implied warranties of merchantability and fitness for a particular purpose. Advanced Chemistry Development, Inc., shall not be liable for errors contained herein or for any direct, indirect, special, incidental, or consequential damages in connection with the use of this material.

Table of Contents

Before You Begin	ii
About this Tutorial	ii
Mouse Conventions	ii
For More Information.....	iii
<i>How to Contact Us.....</i>	<i>iii</i>
<i>Online Updates</i>	<i>iii</i>
1. Introduction.....	1
1.1 About ACD/Structure Drawing Applet	1
1.2 Related Software.....	2
2. Drawing Simple Structures.....	3
2.1 Objectives	3
2.2 Drawing Atoms and Bonds.....	3
2.2.1 <i>Using the Draw Normal Tool.....</i>	<i>3</i>
2.2.2 <i>Double and Triple Bonds.....</i>	<i>4</i>
2.2.3 <i>Deleting Atoms Individually</i>	<i>4</i>
2.2.4 <i>The Undo Command.....</i>	<i>5</i>
2.2.5 <i>Polymers.....</i>	<i>5</i>
2.2.6 <i>Markush Bonds</i>	<i>7</i>
2.2.7 <i>Changing the Atom.....</i>	<i>8</i>
2.2.8 <i>Using Mouse Drag.....</i>	<i>9</i>
2.2.9 <i>Cleaning the Structure.....</i>	<i>9</i>
2.2.10 <i>Using the Stereo and Undefined Bond Tools.....</i>	<i>10</i>
2.3 Selecting Structure Fragments.....	10
2.4 Zooming In/Out on a Structure.....	11
2.5 Input/Output	11
2.5.1 <i>Embedding the Structure in a Document.....</i>	<i>11</i>
2.5.2 <i>Copying/Pasting the Structure as Mol Text.....</i>	<i>11</i>
2.6 Clearing the Screen	11
3. Drawing More Complex Structures and Reactions	12
3.1 Objectives	12
3.2 Using the Radicals Table	12
3.2.1 <i>Creating the Structure of Benzenesulfonic Acid.....</i>	<i>13</i>
3.3 Using the Templates Window	14
3.3.1 <i>Creating Ring Structures.....</i>	<i>14</i>
3.4 Deleting Atoms and Fragments.....	15
3.4.1 <i>Deleting Several Atoms Simultaneously</i>	<i>15</i>
3.5 Replacing Atoms	16
3.6 Setting Double and Triple Bonds	16
3.7 Setting Charges and Defining Anions and Cations	16
3.8 One More Example: Creating the Structure of Testosterone	17
3.9 Drawing a Single-Step Reaction	19

Before You Begin

Thank you for purchasing ACD/Structure Drawing Applet. We have endeavored to produce a very light and functional, platform-independent structure drawing tool.

About this Tutorial

This tutorial provides a comprehensive description of all the drawing facilities available in the ACD/Structure Drawing Applet, 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 the other properties of the window elements described throughout the tutorial correspond with the default Windows Display Properties.

This tutorial is provided in electronic form, readable with a commonly available word processing program. If you cannot locate an index topic you need in the online Help, please do a text string-search in the word processing program for the relevant word or phrase, or related words.

Mouse Conventions

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

- **Point to** means move the mouse pointer to an item.
- **Click** or left-click means point to an item, and press the left mouse button.
- **Right-click** means point to an item, and press the right mouse button.
- **Double-click** means point to an item, and quickly press the left mouse button twice.
- **Drag** means point to an item, press and hold down the left mouse button while you move the item.
- **Select** means highlight or make active an interface element 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 clear, without a mark).

For More Information...

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

<http://www.acdlabs.com>

Our Web site is being accessed at the rate of tens of thousands of “hits” per day. There’s a reason for this: much is offered through our Web site. As of Spring 2004, we offer free ChemSketch 5.0, a free ISIS 3D Add-in, free CambridgeSoft 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 Studio-based movies which show the operation of many of our software packages (especially ChemSketch) available for download.

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

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

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

If you would like to partake of the ChemSketch newsgroup, please access:

<news://news.acdlabs.com/acd.public.chemsketch>

How to Contact Us

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

info@acdlabs.com

Technical and scientific support issues should be addressed by visiting:

<http://support.acdlabs.com>

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

Online Updates

Version 5.0 and later of all PC-based ACD/Labs software contains the capability to have software updates delivered online. You will need the registration numbers of the software and an Internet connection from the same computer on which the software is installed. The updates are small fixes, for example, bringing the actual version number of a program from 8.00 to 8.01. Please refer to the document, "Online Updates," included with the rest of the product documentation in your Documents folder for more information on this, or e-mail our technical support department.

1. Introduction

1.1 About ACD/Structure Drawing Applet

Welcome to ACD/Structure Drawing Applet (ACD/SDA). This is a complete structure drawing, editing, and visualization tool written in pure Java that can be incorporated into HTML documents. The applet can be used for composing substructure queries to databases and visualizing results. Unlike platform-dependent plug-ins or ActiveX controls, the applet runs in the same way on any hardware platform or operating system—the only requirement is a Java-compatible browser such as Netscape 4.0 or later or Microsoft Internet Explorer 4.0 or later.

ACD/Structure Drawing Applet can be used to create true platform-independent Web applications ranging from electronic conferences to online database searches. ACD/SDA is featured in ACD/Web Librarian and ACD/I-Lab.

ACD/Structure Drawing Applet is fully compatible with JDK 1.3.0 specifications, but may also run in a browsers' built-in Java Virtual Machine.

ACD/Structure Drawing Applet is a “chemically intelligent” applet. It understands valency and atom charges, and sets them automatically as you draw your structure. If you make a mistake, the applet will show you where.

The main features of the applet are:

- ⇒ Drawing of any atom from the periodic system with or without a charge;
- ⇒ Ability to change valence, charge, and isotope for a chosen atom;
- ⇒ Ability to replace any atom in a structure with a label;
- ⇒ Drawing of single, double, and triple bonds;
- ⇒ Drawing stereo bonds;
- ⇒ Drawing Markush bonds;
- ⇒ Drawing polymers;
- ⇒ Drawing single-step chemical reactions;
- ⇒ Automatic accounting of hydrogen atoms according to a heavy atom's valency and charge;
- ⇒ Moving and erasing selected parts of the structure or the whole structure;
- ⇒ Undo and redo functions;
- ⇒ Zooming in and zooming out;
- ⇒ Predefined molecular templates;
- ⇒ Ability to add customized molecular templates;
- ⇒ Loading a structural fragment from the built-in table of radicals;
- ⇒ Drawing query atoms and bonds;
- ⇒ Ability to attach templates to an atom or bond;

- ⇒ Docking and Floating modes;
- ⇒ Exporting/importing the drawn structure into/from MDL Molfile format;
- ⇒ Loading a structure into the applet from the server;
- ⇒ Loading a structure into the applet by a JavaScript function call;
- ⇒ Composing substructure queries based on a drawn structure;
- ⇒ Removable toolbars for maximum structure visualization area;
- ⇒ 2D molecule optimization (Clean) function for normalizing your molecular drawing even for structures including several Markush bonds (server support required); and
- ⇒ Copying/pasting image as mol text and image to/from Windows Clipboard.

1.2 Related Software

ACD/Web Librarian gives your chemists and analysts the resources and tools necessary to perform these tasks in an efficient manner. Web Librarian is an enterprise solution that offers your organization a fully customizable, browser-based service for viewing ACD/Labs databases.

With **ACD/Web Librarian**, your chemists and analysts can optimize their valuable time by gaining unified access to structure and spectra data collected throughout the enterprise. Data is displayed in a virtual, centralized repository that is accessible to authorized members of the organization. Furthermore, Web Librarian provides a collaborative framework for sharing analytical record data to ensure that accurate information is available to all members of a project team. This not only speeds up their research and analysis, but also eases information retrieval and creates an efficient work environment in order to make effective mission-critical decisions.

ACD/Labs Online (I-Lab), the Interactive Laboratory, is an Internet-based service for instant access to chemical databases and property predictions programs. Since 1996 it has gained a reputation as one of the most innovative online services for prediction. With over three thousand users worldwide, I-Lab is being successfully used for teaching chemistry in several leading American universities as well.

With **I-Lab online access**, you can:

- Search databases by structure and substructure;
- Obtain NMR spectra;
- Generate systematic chemical names for your molecules; and
- Predict properties such as pK_a , $\log P$, or solubility for the chemical structures.

You can get these facilities from both your Internet browser and from inside ACD/ChemSketch (with ACD/I-Lab Add-on for ChemSketch 5.0 installed), a powerful *structure drawing tool* that can be downloaded from our Web site FOR FREE.

We do offer a two week demonstration period for **new I-Lab users**. The demonstration period enables you to use all I-Lab services free of charge for two weeks. To make use of this offer, visit us now at:

<http://www2.acdlabs.com/ilab>.

2. Drawing Simple Structures

2.1 Objectives



The objective of this chapter is to give you an overview of the chemical drawing features of SDA. You will learn how to:

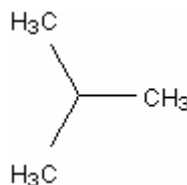
- Draw atoms, bonds (single, double, triple, wedge, undefined, and Markush), and polymers;
- Select and resize drawn structures;
- Generate stereo descriptors; and
- Clear the screen.

2.2 Drawing Atoms and Bonds

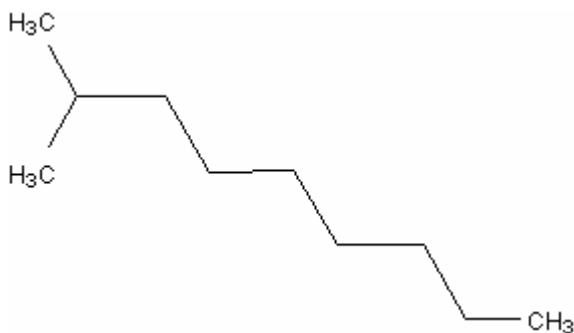
2.2.1 Using the Draw Normal Tool

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

1. Make sure that the **Draw Normal** tool  is enabled on the Structure toolbar and that the **Carbon** atom  is selected on the Atoms toolbar.
2. Click in an empty space to draw CH₄.
3. Click the CH₄ carbon to add a —CH₃ group, creating CH₃—CH₃ with a standard bond length. Click the same carbon twice more to draw:

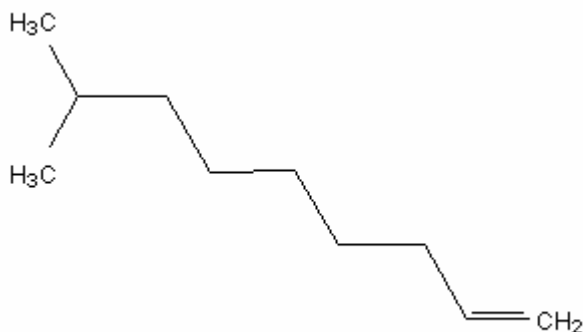


4. In the **Templates** pop-up window, open **Chains (saturated)** and select the **C6** chain by clicking the leftmost carbon atom of the C6 fragment, and then click the rightmost carbon of our structure to draw

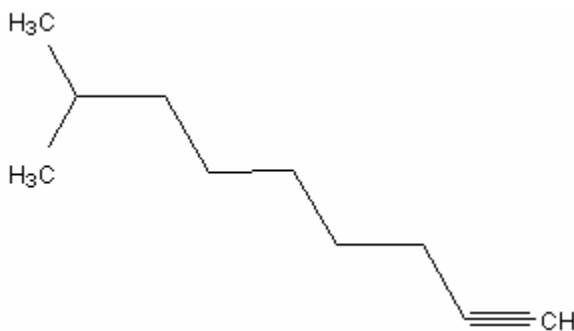


2.2.2 Double and Triple Bonds

1. On the last structure drawn, hover over the terminal bond until it is highlighted and then click once to convert it to a double bond:



2. Click again to convert it to a triple bond:

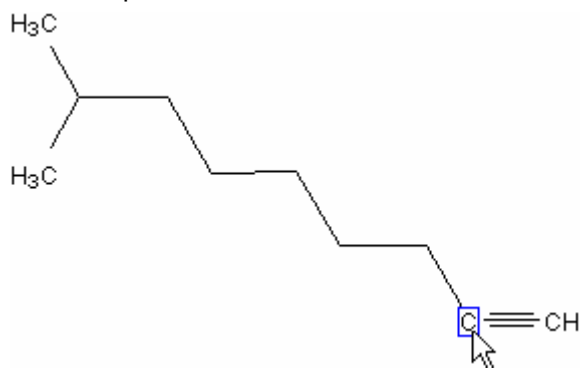


3. Click again to convert it back to single bond.

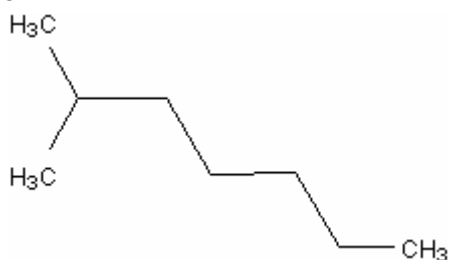
2.2.3 Deleting Atoms Individually

If you have added too many atoms, you can remove them.


1. Click **Delete** .
2. Click the atom highlighted in the picture:



The molecule now looks like this:

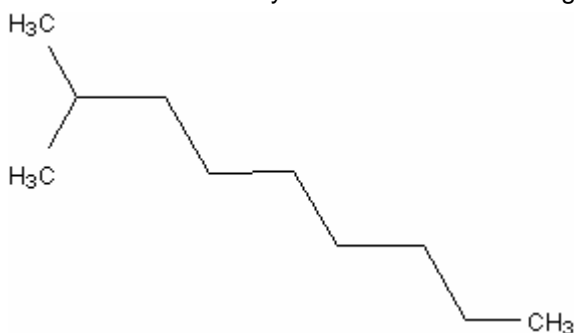


2.2.4 The Undo Command

Another important operation is the **Undo** command. Click **Undo** , and the SDA screen will revert to exactly what it was before your last change.

Note As soon as the **Undo** button is clicked, the **Redo** button becomes active.

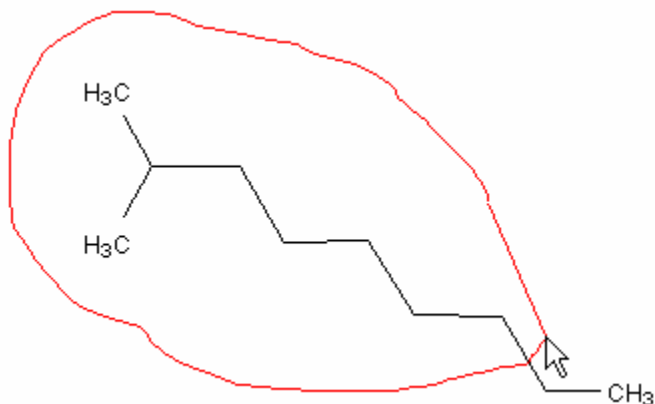
Click the **Undo** button several more times until you return to the following structure:



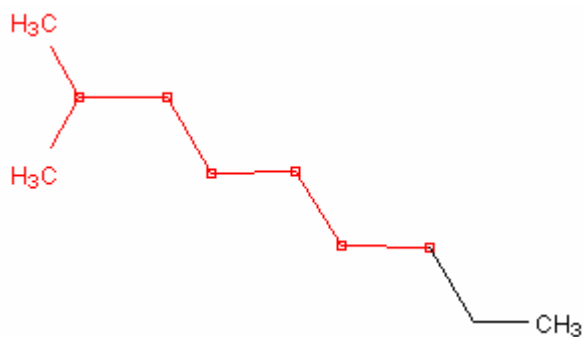
Note The **Undo** command can be repeated up to 7 times. When you begin to draw more complex molecules or graphical objects, we recommend that you develop a habit of saving your work to a file after making several changes.


2.2.5 Polymers

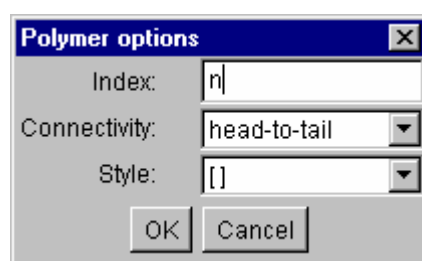
1. Left-click and drag to include all of the specified atoms in the closed Lasso line to select them:



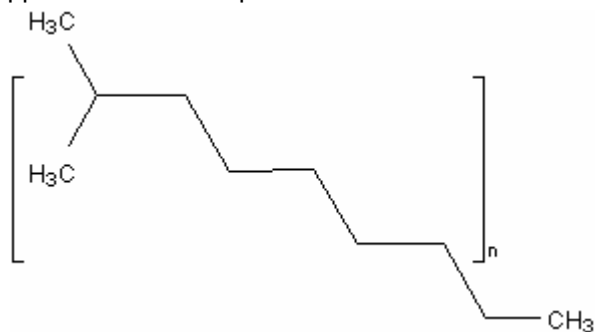
2. Release the mouse button. The fragment inside the Lasso line becomes selected:



3. Click **Polymers**  on the Structure toolbar to display the **Polymer options** panel, and then change the settings as shown:





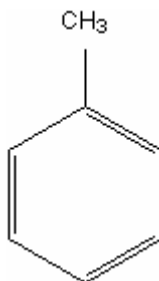
The polymer structure appears in the workspace:






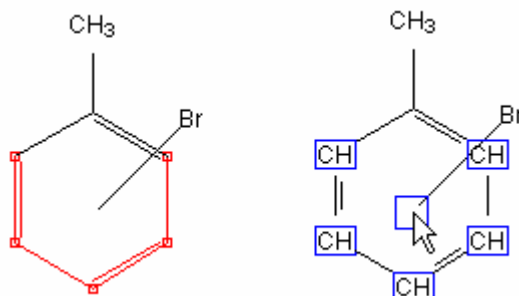
2.2.6 Markush Bonds

To denote structures with an undefined attachment point, use the Markush bond tool.

1. In the **Radicals Table** dialog box, select benzene, and then click in the workspace.
2. Make sure that the **Draw Normal** tool  is enabled on the Structure toolbar and that the **Carbon**  atom is selected on the Atoms toolbar.
3. Click the topmost atom of benzene to sprout the methyl group:



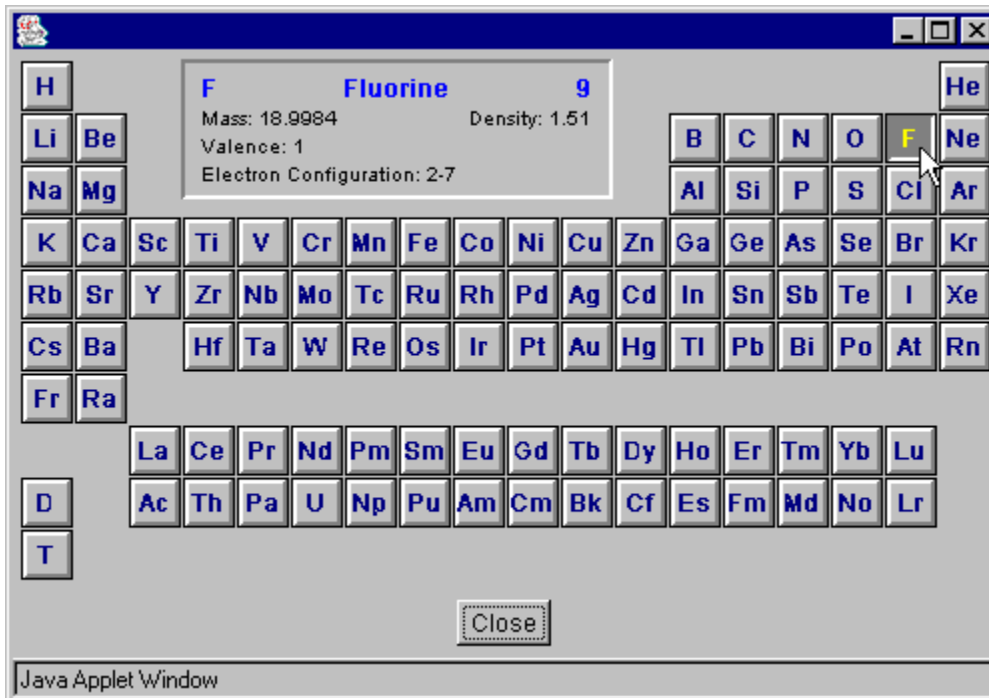
4. On the Atom toolbar, select **Bromine**  to attach it with a Markush bond.
5. Select the five CH atoms of the structure using the **Select/Move** tool .
6. On the Structure toolbar, click **Markush Bond** . The selected element connected by the Markush bond appears:




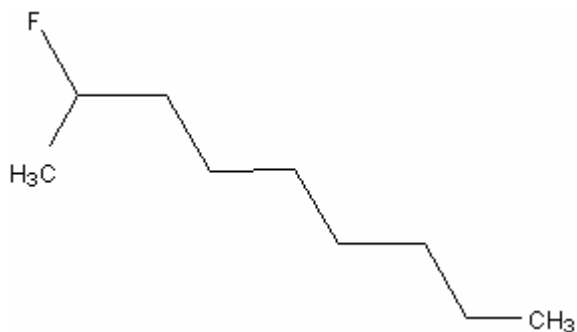
Note In this structure, bromine atom might be connected to any one of the five carbon atoms of toluene. All five carbon atoms are highlighted by moving the mouse pointer over to the variable attachment point of the Markush bond.

2.2.7 Changing the Atom


1. On the Atoms toolbar, click **Periodic Table**  to open the **Periodic Table of Elements**:



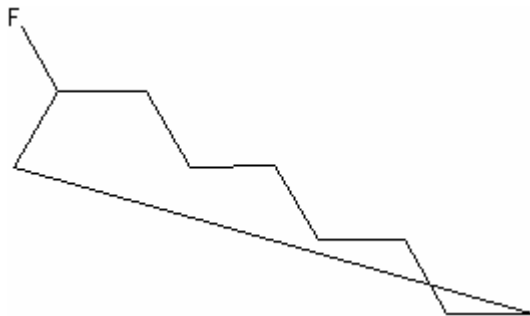
2. In the Periodic Table of Elements, click **Fluorine** . The **Fluorine** button now appears on the Atoms toolbar.
3. Click the left-most carbon atom to replace it with a fluorine one:



2.2.8 Using Mouse Drag


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

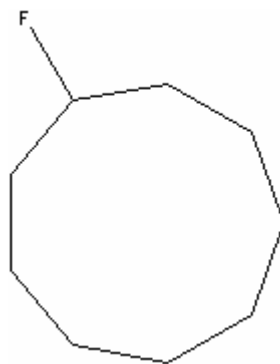
With the **Draw Normal** tool active, point the mouse arrow to one of the terminal carbons and drag to another terminal carbon to draw the following structure:



2.2.9 Cleaning the Structure

Important The **Clean** tool works with the help of external “cleaning” software present when ACD/SDA is launched from ACD/Web Librarian or ACD/I-Lab.




On the Structure toolbar, click **Clean**  to standardize all the bond lengths and angles in the drawn structure to obtain the following image:



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

2.2.10 Using the Stereo and Undefined Bond Tools

Click the bottom-right triangle of the **Draw Normal** button  on the Structure toolbar to expand it to the following group:

-  Draw Normal
-  Draw Up Stereo
-  Draw Down Stereo

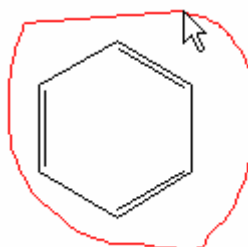
You can draw a wide variety of chemical bonds:


Select any of these tools and click any bond in the drawn structure. Click repeatedly on a stereo or coordination bond to change its direction. Click once more to change the bond to the undefined type (without definite direction).

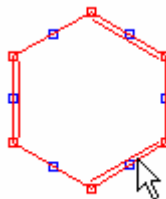
2.3 Selecting Structure Fragments

You can select atoms, bonds, and other fragments of your molecular structure or reaction scheme:



- On the Structure toolbar, click **Select/Move** . In the Drawing area, click and drag to include all of the specified atoms of your structure in the closed Lasso line to select them:





Release the mouse button. Once the fragment(s) has been selected, you can move it as the **Select/Move**  tool is active:




Additionally, you can perform other operations with the selection as well using the corresponding tools:

- Delete** . For more information, refer to Section 2.2.3.
- 2D Optimization** (or **Clean**) . For more information, refer to Section 2.2.9.

2.4 Zooming In/Out on a Structure


You can zoom in/out on the structure by clicking **Zoom In/Out**  . If the structure is larger than the Drawing area you may scroll it with the help of scroll bars.

To zoom a structure to fit completely in the window, click **Fit to Page** .


2.5 Input/Output


2.5.1 Embedding the Structure in a Document

Sometimes you need to insert the structure into a report written in different applications (e.g., Microsoft Word document, Excel spreadsheet, etc.).

1. Select the required structure(s).
2. Click **Copy as Image**  to copy the selection to the Clipboard.
3. Switch to the application where you want the structure(s) to be inserted, and paste using the Paste function of that application.



2.5.2 Copying/Pasting the Structure as Mol Text

To copy the contents of the Drawing area as mol text, click **Copy as Mol Text** .

To paste a structure stored as mol text from the clipboard to the Drawing area, click **Paste from Mol Text** .

2.6 Clearing the Screen

To clear the screen, you can do one of the following:

- From the Structure toolbar, click **Clear** .
- On the Structure toolbar, click **Delete** . Click in an empty space away from the drawn structure to select all of the structures, and then click any structure to delete the entire screen.

3. Drawing More Complex Structures and Reactions

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/Structure Drawing Applet.

In this chapter you will learn how to:

- Use the Radicals Table to draw typical chemical fragments;
- Use Templates to move a step closer to advanced drawing expertise;
- Delete and replace atoms;
- Set double and triple bonds;
- Set an atom's charge, and draw cations and anions; and
- Draw single-step chemical reactions.

3.2 Using the Radicals Table

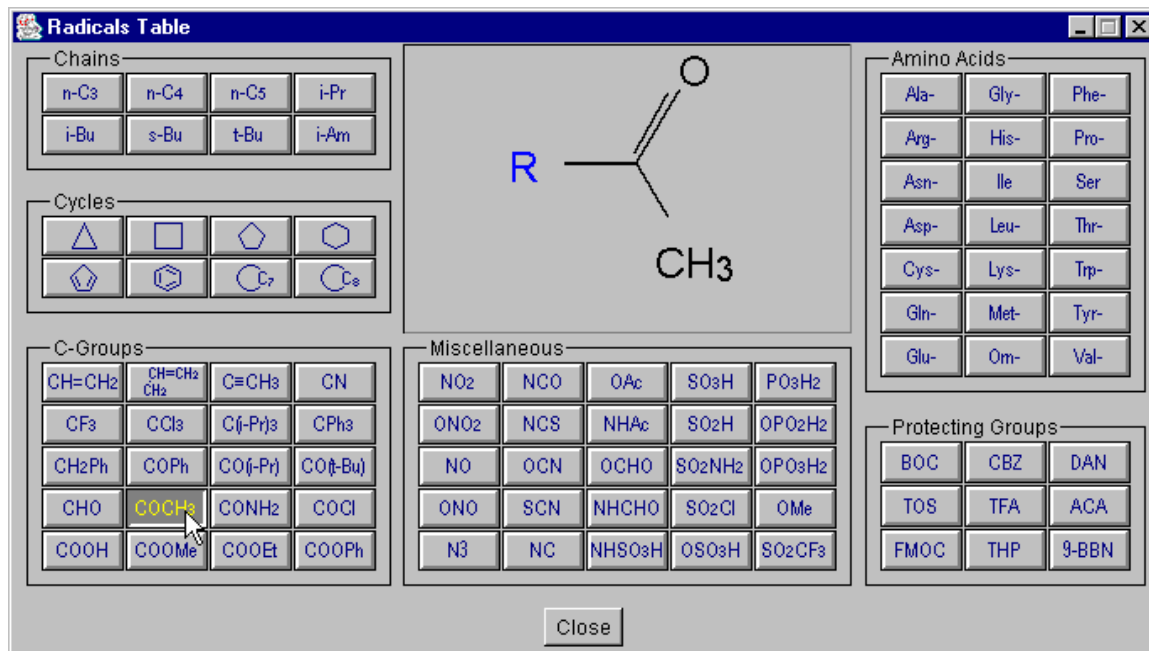
ACD/Structure Drawing Applet includes the following two structure template tools:



- **Radicals Table** dialog box 
- **Templates** window 

The **Radicals Table** is a set of chemical radicals for structure drawing. It includes structures of amino acids, their protecting groups, as well as nucleotides and other frequently used radicals. Their names and, in some cases, abbreviations are listed to help you quickly translate "chemistry shorthand" into a meaningful molecule.

1. Clear the screen using the directions given in previous section.

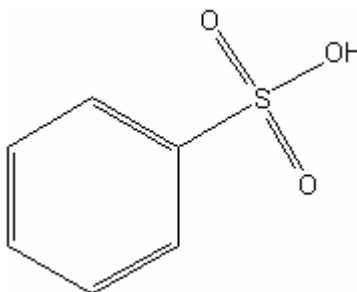
2. On the References toolbar, click **Radicals Table**  to open the **Radicals Table** dialog box:





3. In the **Radicals Table** dialog box, click **Benzene**  to select the structural element and return to the ACD/SDA window
4. A Benzene button is now located and currently selected on the References toolbar on the right side of the screen.
5. Repeat these steps for **Sulfo** .

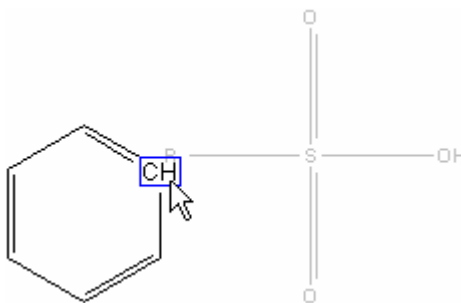
Note When you select new radicals from the Table of Radicals, the corresponding buttons are automatically added to the References toolbar.

3.2.1 Creating the Structure of Benzenesulfonic Acid



1. Delete all structures.
2. Click **Benzene**  on the References toolbar on the right side or select it from the **Radicals Table**.
3. Click in the Drawing area to copy the structure.
4. On the same toolbar, click **Sulfo** .

5. Click any atom to place the radical:



3.3 Using the Templates Window

While the binding point of any template in the **Radicals Table** dialog box is fixed (invariable), the **Template** window allows you to specify any atom or bond to be the binding point simply by clicking directly on it. However, no matter what the source of the template is, the principles of joining are the same.

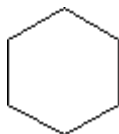
There are several ways of joining the template to a drawn structure:

- **By fusing the bonds of the structure and template:** point the mouse cursor over the bond so that the corresponding bonds of the structure and template shadow are fused and then click.
- **By attaching the template to the structure:** point to the corresponding atom on the structure so that the connecting bond appears, and then click.

3.3.1 Creating Ring Structures

1. Click **Templates** . In the following **Templates** window, click **Rings**, and then click any

atom or bond of the **Cyclohexane** structure




2. Click in the Drawing area workspace to copy the template.

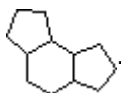
3. In the **Templates** window, click **Rings**. Point to any bond of the **Cyclopentane** structure



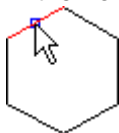
, and then click it.

4. Now sequentially point to the indicated bonds  to highlight, and then click them to

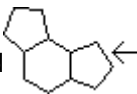
create the following structure:

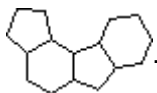





5. In the **Templates** window, click **Rings**. Point to any bond of the **Cyclohexane** structure,

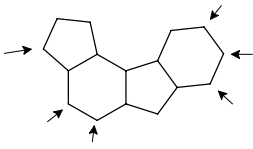


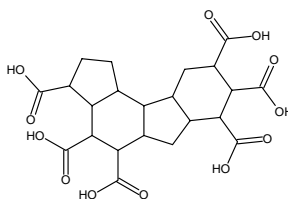
and then click it.

6. Point to the indicated bond  to highlight, and then click it to create the following structure:

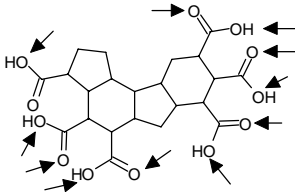
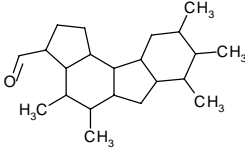


7. Click **Radicals Table**  on the References toolbar.
8. In the **Radicals Table** dialog box, select the carboxyl group  by clicking **Carboxyl** .

9. Click the atoms indicated in the structure  to sprout carboxyl groups out of them:




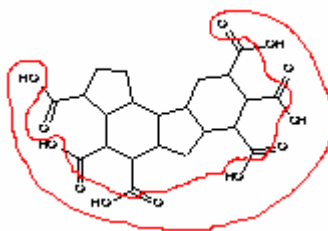
3.4 Deleting Atoms and Fragments

- Delete the atoms indicated by arrows in  to draw 

You can do this in two ways: delete each atom individually (for more information, refer to Section 2.2.3) or delete several atoms simultaneously.

3.4.1 Deleting Several Atoms Simultaneously

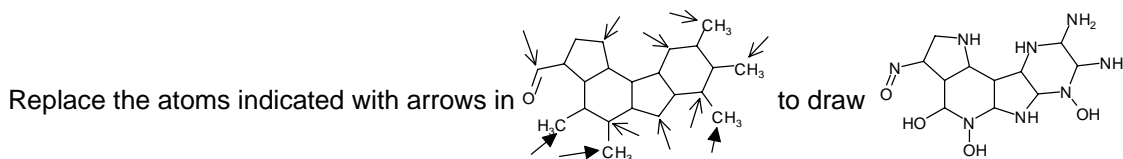
- On the Structure toolbar, click **Move** .
- Drag to include all of the specified atoms in the closed Lasso line to select them:





- On the Structure toolbar, click **Delete** .
- Click any one of the highlighted atoms to delete all of them simultaneously.

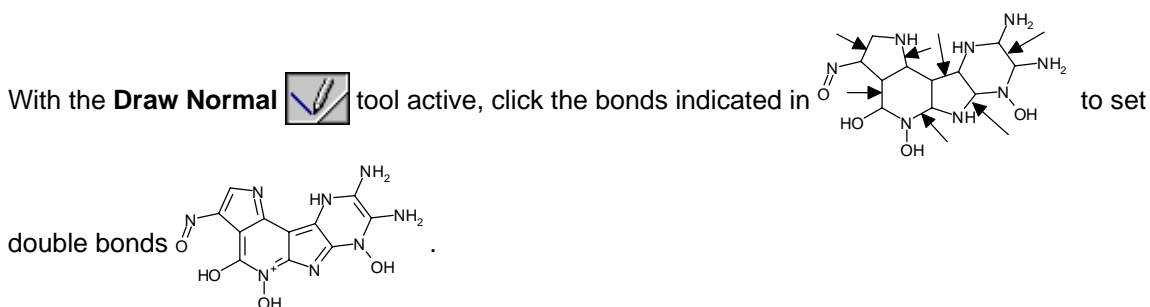
Note To deselect all fragment(s), click anywhere in an empty space.

3.5 Replacing Atoms



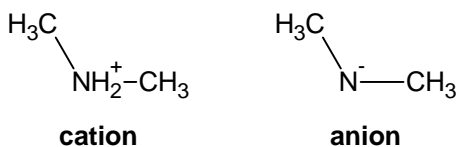
1. On the **Atoms** toolbar, click **Nitrogen** , and then click all the carbons denoted by an open-head arrow on the above structure.
2. On the **Atoms** toolbar, click **Oxygen** , and then click the three Carbons denoted by a solid-head arrow.



3.6 Setting Double and Triple Bonds

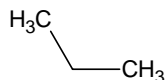



3.7 Setting Charges and Defining Anions and Cations

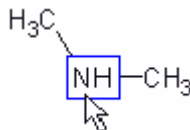
In this section we will draw the following set of structures:




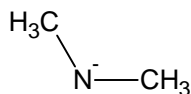
1. Click **Carbon**  on the Atoms toolbar and make sure that the **Draw Normal** tool  is on. Click three times in one place to draw the following structure:




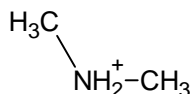
2. Click **Nitrogen**  and click the middle carbon in the fragment to replace it with a nitrogen:





3. Click **Charge Minus**  and then click the NH group to make an anion:

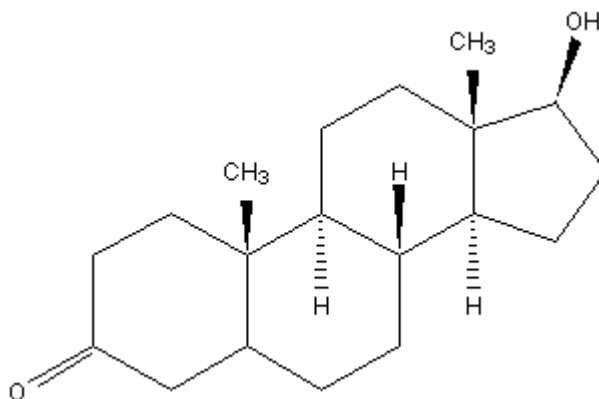



4. Click **Charge Plus** , and then click twice to make a cation:



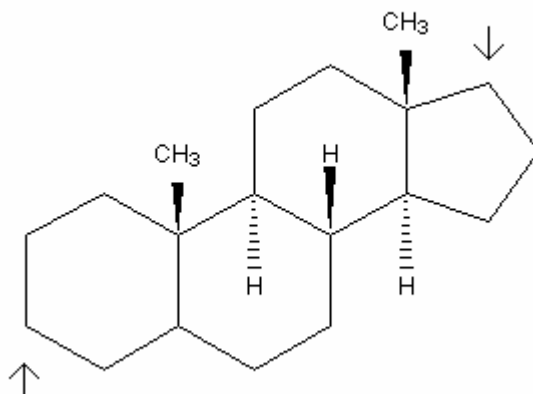
Note When you use the **Charge** buttons,  or , to change the charge of a nonmetal, the corresponding number of hydrogen atoms is automatically added to it, or removed from it, to preserve proper chemical valency. If you change the charge of a metal, the charge is changed in increments or decrements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

3.8 One More Example: Creating the Structure of Testosterone

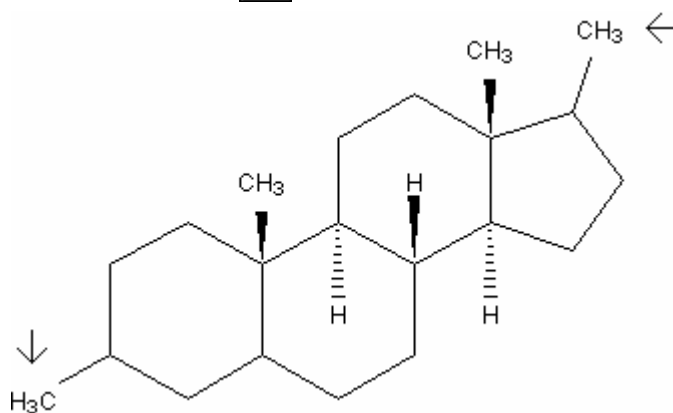


1. Delete all structures.
2. Click **Templates** .
3. In the following **Templates** window, click **Steroid(1)**, and then click the **androstane** structure.
4. Click in the Drawing area workspace to copy the template.

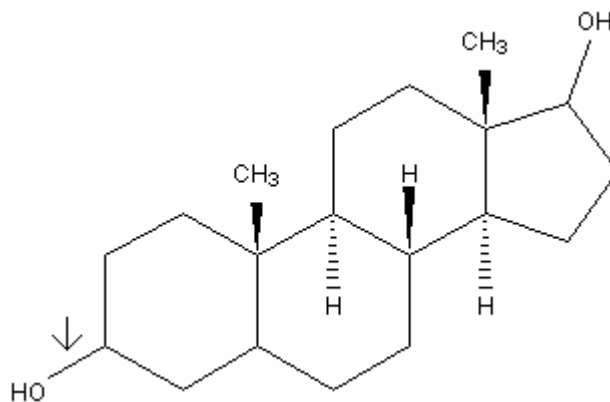
5. On the Atoms toolbar, click **Carbon** , and then click the indicated atoms:





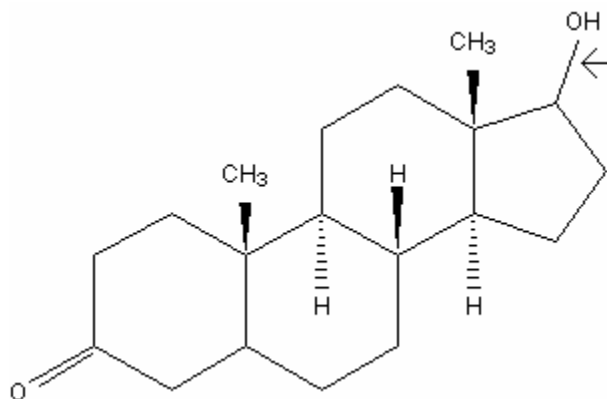
6. On the Atoms toolbar, click **Oxygen** , and then click the indicated atoms:



7. Click the indicated bond:

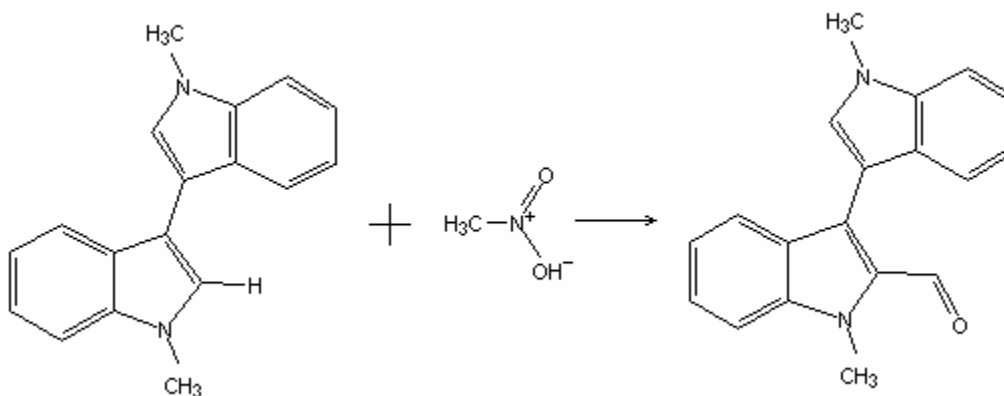



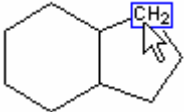
8. Click the bottom-right triangle of the **Draw Normal** button  on the Structure toolbar, and then click **Draw Up Stereo** .
9. Click the indicated bond:



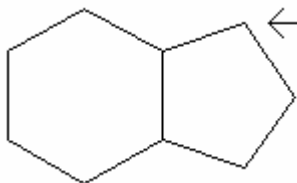
3.9 Drawing a Single-Step Reaction


In this section, we will draw the Vilsmeier Formylation reaction:

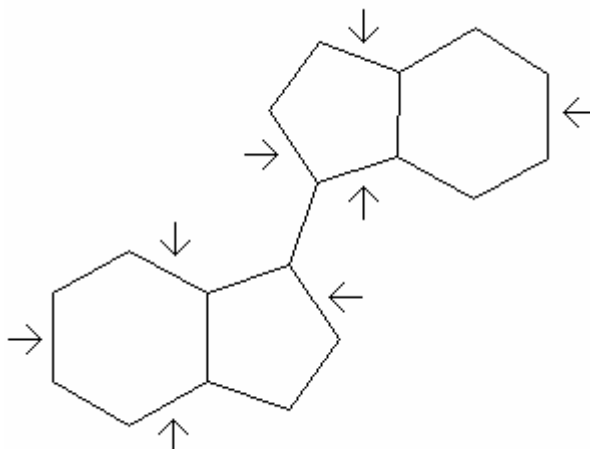



1. Click **Templates** . In the following Templates window, click **Polycyclics**. Point to the indicated atom of the **Hydryndane** structure , and then click it.

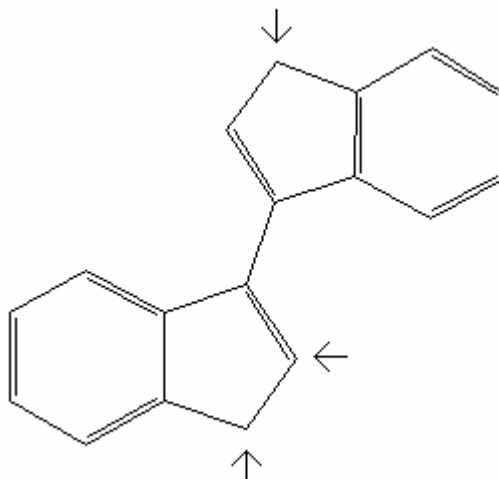
2. Click in the Drawing area workspace to copy the template.
3. Point to the indicated atom of the drawn structure, and then click it:



4. With the **Draw Normal**  tool active, click the bonds indicated in the following image to set double bonds:

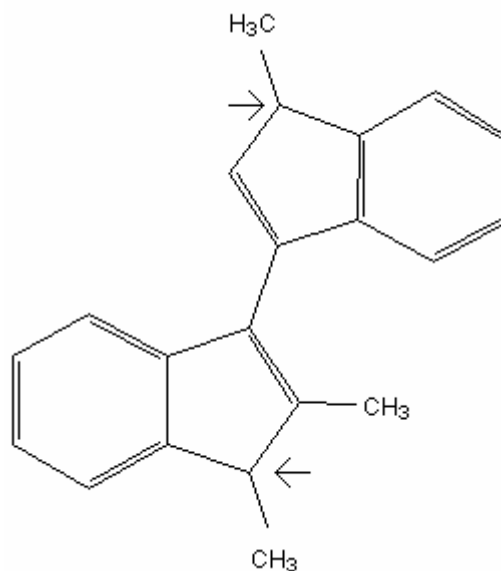


5. Make sure that the **Carbon** atom  is selected on the Atoms toolbar.
6. Click the indicated atoms to add CH₃ groups:



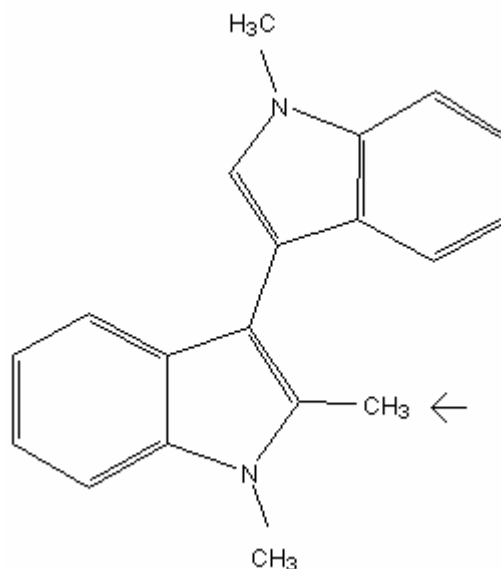
7. On the **Atoms** toolbar, click **Nitrogen** .

8. Click the indicated atoms to replace them with nitrogen atoms:



9. On the **Atoms** toolbar, click **Hydrogen**

10. Click the indicated atom to replace it with a Hydrogen atom:




11. On the Structure toolbar, click **Select/Move** , and then click in an empty space away from the drawn structure to select it.

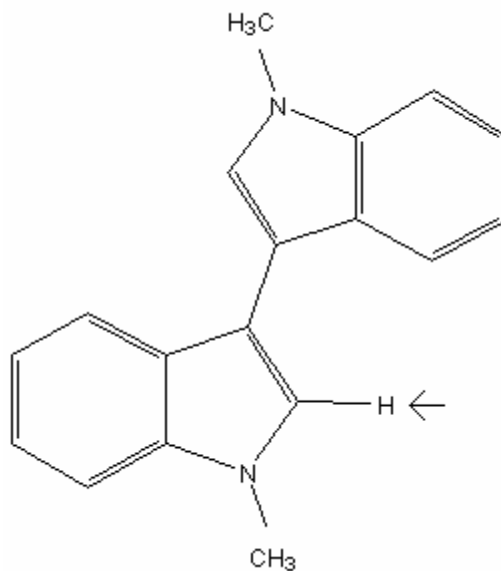
12. Click any atom or bond of the structure, and then drag it to the right part of the drawing area.

13. On the Structure toolbar, click **Copy as mol text** , and then click **Paste from mol text**




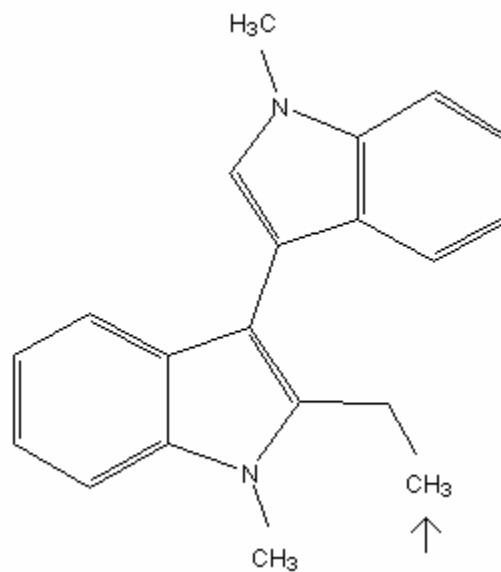
; a copy of the structure appears in the left part of the drawing area.

14. On the **Atoms** toolbar, click **Carbon** , and then click the indicated atom of the right structure to replace it with a carbon atom:

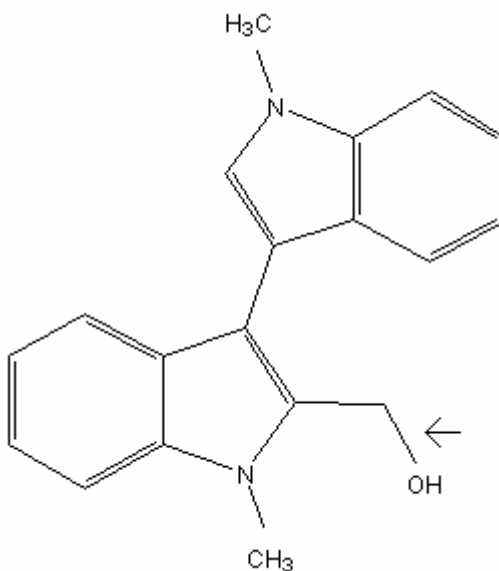



15. Click that atom again to add a methyl group.


16. On the **Atoms** toolbar, click **Oxygen** , and then click the indicated atom of the right structure to replace it with an oxygen atom:



17. Click the indicated bond of the right structure to set a double bond:

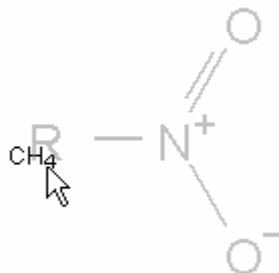


18. On the **Atoms** toolbar, click **Carbon** , and then click in an empty space between the drawn structures to draw CH₄.

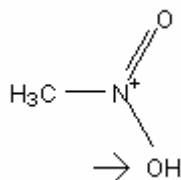
19. On the References toolbar, click **Radicals Table** .

20. In the **Radicals Table** dialog box, click **Nitro** .


21. Click the drawn CH₄ to place the radical:

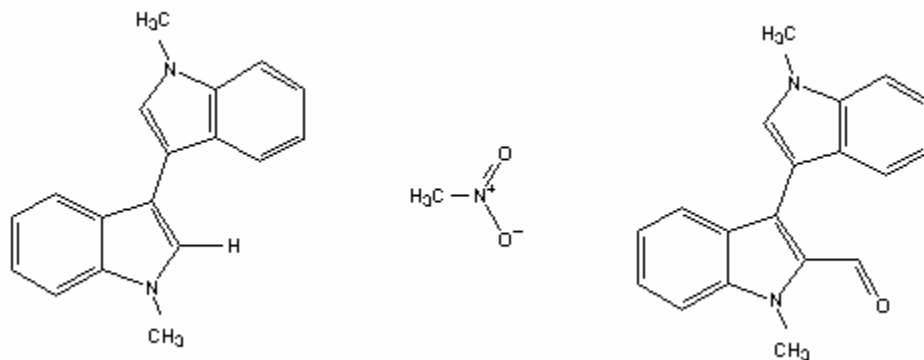


22. On the Structure toolbar, click **Charge Minus** , and then click the indicated atom:



23. On the Structure toolbar, click **Zoom Out**  several times to get enough empty space in a drawing area to place the reaction.

24. Rearrange the drawn structures as shown in the following image using **Select/Move** :



25. Insert a reaction plus and a reaction arrow into corresponding places between the structures.
The reaction scheme is finished.