



## Experiment 19

### ChemDraw Tutorial and Assignment

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ChemDraw is the chemical structure drawing program most frequently used by organic chemists. Most of the chemical structures that you see in texts, journal articles, and on the web were drawn in ChemDraw. If you learn the basics of this program now, you can use it to prepare written reports and power point presentations during the rest of your university career (and beyond).

Besides drawing structures, ChemDraw is also useful for:

- Naming a compound.
- Determining the structure of a named compound.
- Predicting the NMR spectrum of a compound.
- Finding physical data.
- Finding the molecular weight of fragments for mass spectroscopy.

ChemDraw is available on all of the computers in the organic chemistry area; feel free to come use it at any time that the labs are open. For home use, you can go to the CambridgeSoft web site\* and download a free trial version of ChemDraw Ultra 8.0. If you want to purchase ChemDraw, an academic version costs \$50.

#### Assignment

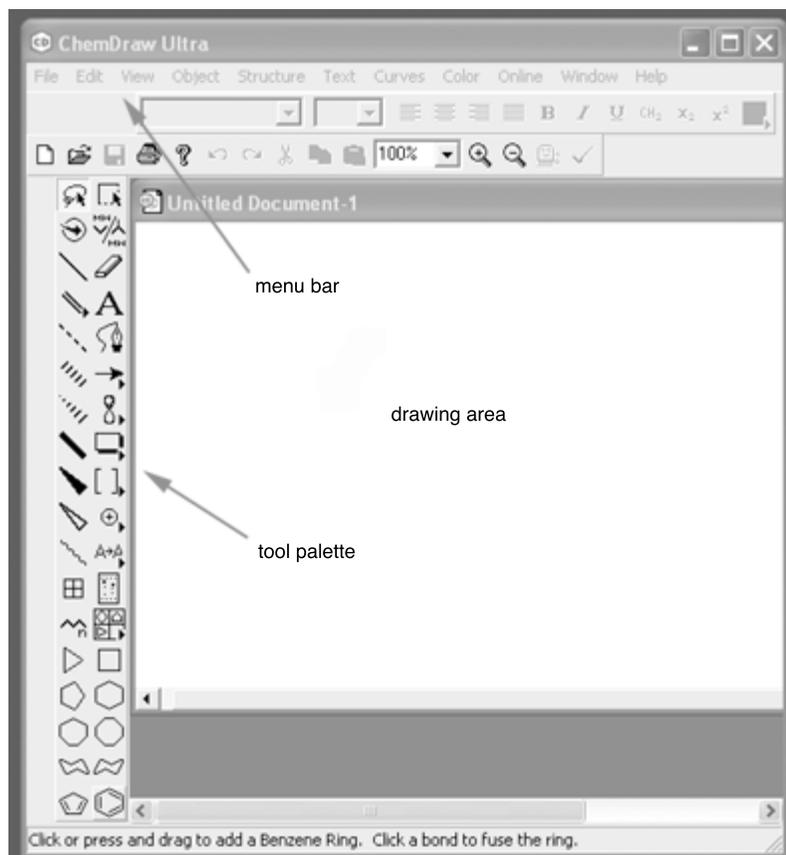
The following exercise is designed to introduce you to the basics of this program. Most of it is practice. The only required parts are marked with “Assignment” and are in sections 9 and 10.

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\* [www.cambridgesoft.com](http://www.cambridgesoft.com)

## 1. Open ChemDraw and choose settings.

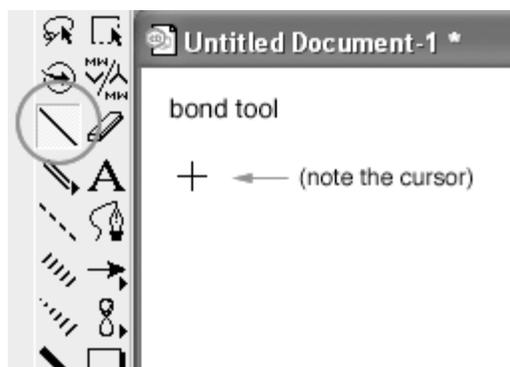
Double click on the *ChemDraw* shortcut or go to the Start menu. Once the program is running, you will see a large drawing area, a tool palette, and the menu bar.



Change the settings to the ACS (American Chemical Society) template: Under the File menu, select “Apply Document Settings from” and choose “ACS Document 1996”. This makes your document look good.

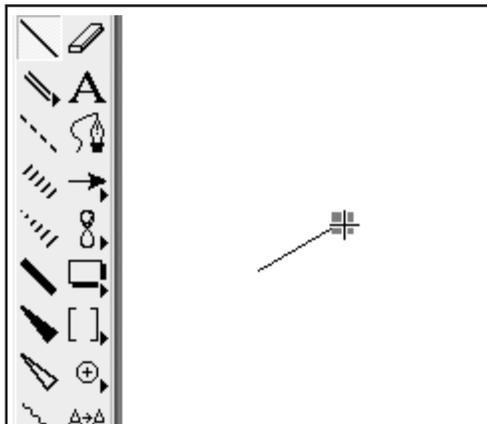
## 2. Drawing using the bond tool.

Click once on the bond tool (“\”), third down on the left in the tool palette. When you click on it, its square will lighten to show it is selected and the pointer will become a crosshair (“+”).



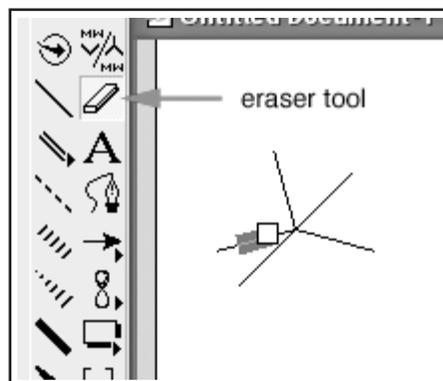
With the bond tool active, click and hold the mouse in the drawing area. Drag the mouse until the bond is orientated how you want it. (You will only be able to draw a bond of a preset length; if you want to draw a line of any length, go to the object menu and un-check “fixed lengths”.)

Once you have one bond drawn, place the cursor on one end of that bond. A black square will appear: this means that you can click and drag again to build another bond onto your “molecule”.



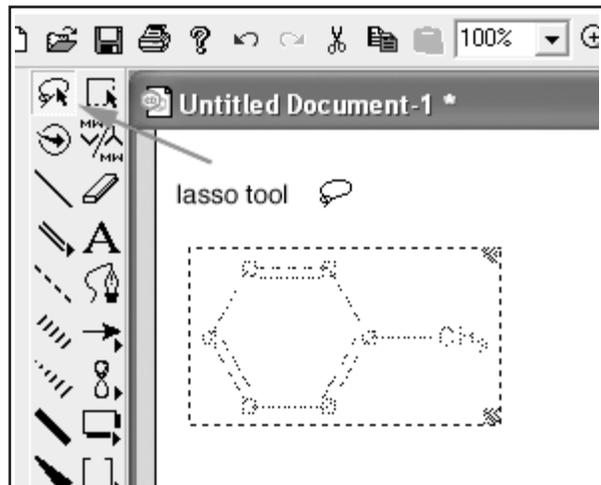
### 3. Fixing mistakes.

Made a mistake? It's okay! Find the eraser—shaped like an eraser and third down on the right in the tool palette. Highlight it, then click on the mistake(s).



Another way to get rid of stuff that you do not want is to select it and backspace. Click on the select tool (shaped like a lasso, upper left in tool palette) and double

click on a structure. When selected, a structure is gray: it sort of “twinkles”. Anything selected can be moved, copied, or deleted.



You can “undo” an action with control-Z.

#### 4. Drawing using the bond tool (con't).

To draw a double bond, with the bond tool selected, trace over a single bond (atom to atom) once to create a double bond. Try this a few times.

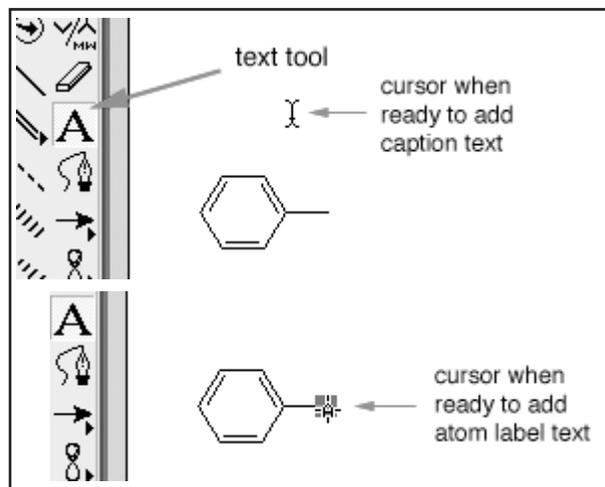
Now try drawing a few molecules.



Note: there is a double bond tool too. Practice using it if you like.

#### 5. Adding atoms.

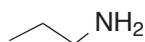
Click on the label tool (looks like an “A”, second column in the tool palette, 4th down). The pointer turns to a thin “I” until you are over any bonding site, then it changes to an “A” in a box.



Click on any bonding site and type in an appropriate atom label. For instance, draw the following ketone:



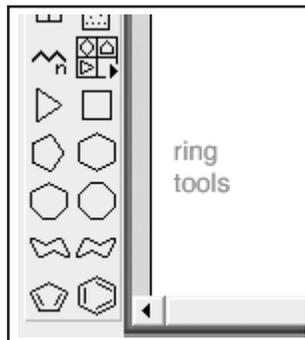
Make sure you hold down the shift key to make it a capital "O". Now draw an amine:



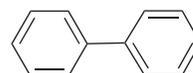
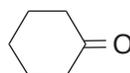
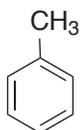
Note how ChemDraw automatically subscripts the "2".

## 6. Rings.

There are several ring tools in the palette. For organic chemistry, you will probably use the aromatic ring and the cyclohexane ring most often.

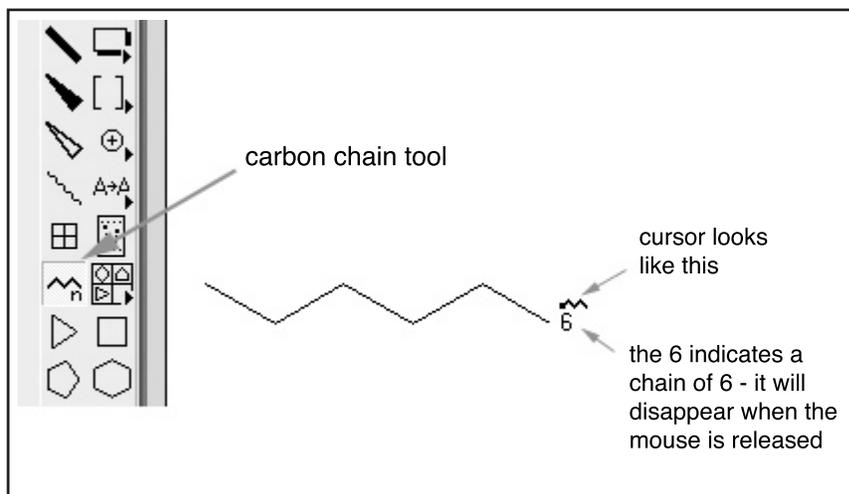


Try the following structures:



## 7. Drawing chains of carbons.

If you need to draw a long chain of carbons, click on the carbon chain tool (see below) and click and drag the mouse across the screen. The end of the chain will have a number after it, indicating how many carbons you have drawn so far.



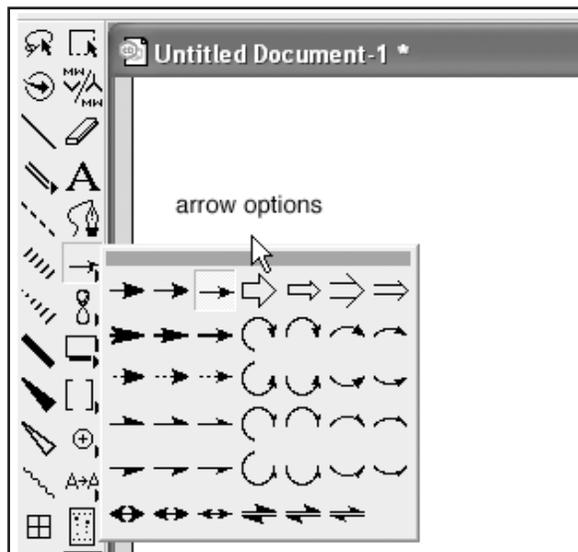
## 8. Adding text (other than atom labels).

Simply click on the same tool described in #5 and click anywhere except on a bonding site. (You have probably already discovered this.)

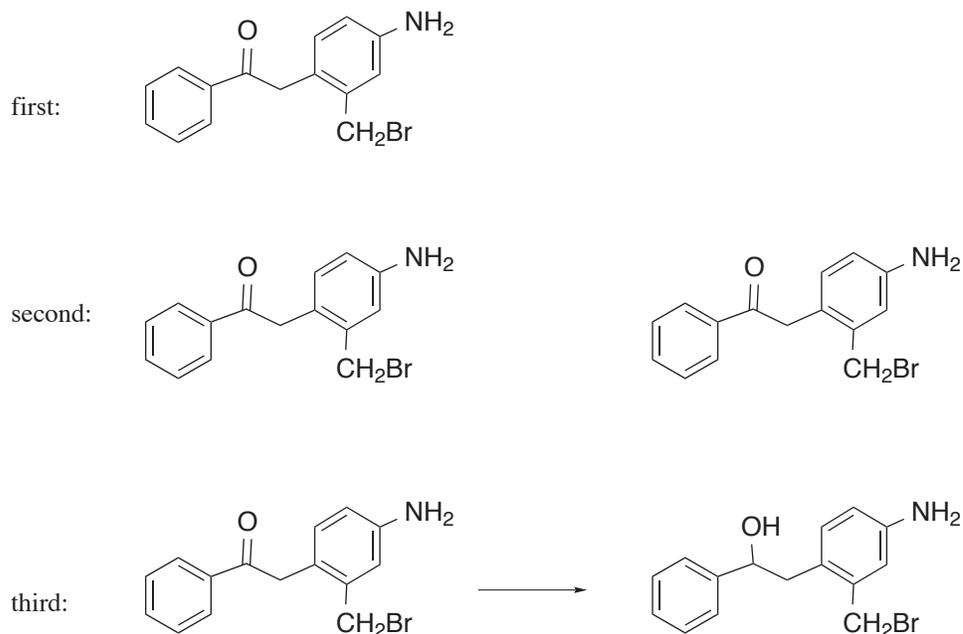
## 9. Drawing reactions.

*Note: Your first assignment is to draw the structures below, print them, and hand them in to your TA.*

Use the arrow tool (looks like an arrow, right column, 6th down) to draw an arrow of any length. The first time you use this tool, you might need to change the type of arrow. Do this by clicking and holding down the mouse, then move to highlight the arrow of your choice.



Often a reaction will involve changing a molecule just a little. Thus, you can draw it once, then copy and paste it to the right of the first structure, then modify the second structure. For instance, draw the complex molecule on the left, select it, copy it, and paste it to the right, move it around if necessary. Modify it to the product. Draw an arrow between the two.

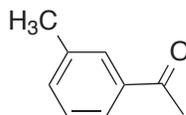


**Assignment:** Draw the above series of structures, including the caption text (“first:”, etc.) and the arrows.

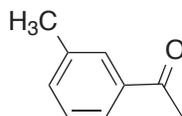
## 10. Naming structures.

*Note: Your second assignment is to draw the structures indicated, have ChemDraw name them (and visa versa), print them, and hand them in to your TA.*

This is a great function. You can draw almost any molecule and ask the program to name it for you. For instance, draw the structure below:



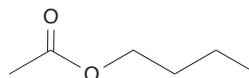
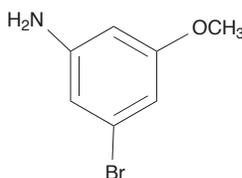
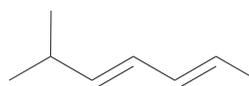
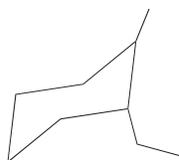
Highlight the molecule (lasso tool, double click on the molecule) and then go to the “Structure” menu. Go down to “Convert structure to name” and the IUPAC name of the compound will appear below the structure:



1-*m*-tolylethanone

You can go backwards too, from name to structure. Type in a compound name, go to the “Structure” menu, and choose “Convert name to structure”.

**Assignment:** Draw the molecules below and have ChemDraw name them for you.



**Assignment:** Type in the names below have ChemDraw name them for you:

- 4-iodo-2-methylphenol
- 4-iodo-*o*-cresol
- phenyl vinyl sulfide
- 5-hydroxy-1-indanone

## 11. Tidying up your structures.

You can align and distribute your drawn molecules to make them look better on the page. Select the structures that you want to work with, then go to the “Object” menu, go down to “Align”, then choose to align left edges, right edges, L/R centers, top edges, bottom edges, or T/B centers. The “Distribute” function is also in the Object menu. Draw a few molecules and practice aligning and distributing them.

## 12. Copying into Word.

To copy your ChemDraw structure or group of structures into Word, copy them to the clipboard, then go to Word and paste them where you want them.

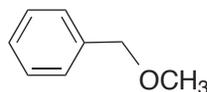
You can also paste ChemDraw structure into PowerPoint. When using PowerPoint, you might want to make your structures colored, or use larger line widths. ChemDraw is pretty intuitive and you can probably figure out how to do this yourself, but if you want help, feel free to ask.

### 13. Saving ChemDraw structures.

You are welcome to save your work—just remember where you put them because the computers in the organic chem area are used by lots of students and at times the hard drives are pretty chaotic. If you put your structures into Word, you can always copy them and then re-open them in ChemDraw.

### 14. Other fun things to do with ChemDraw.

Draw the following molecule:



Highlight it, then go to the “Structure” menu and choose “Predict <sup>1</sup>H-NMR Shifts”.

Go to the “View” menu and choose “Show Analysis Window” and “Show Chemical Properties Window”.

Go to the “Edit” menu and choose “Get 3D Model”.

