

Chemistry 211 / 212, 2005-2006

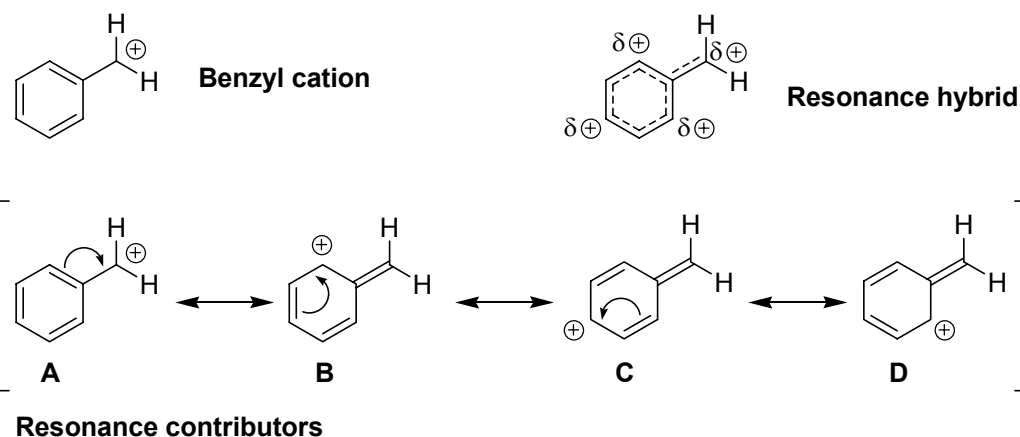
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## ChemDraw Tutorial



CambridgeSoft ChemDraw Pro is a software program used to create professional-quality chemical structures. From now on, all chemical drawings for lab reports and lab report sections must be done with ChemDraw. The program is available in Severance 111 and the Timken Science Library computer classroom. The following tutorial will help you to develop the basic ChemDraw skills necessary to draw the benzyl cation and its resonance structures.



### GETTING STARTED

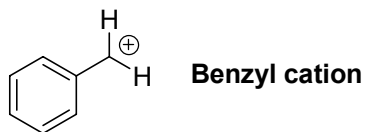
1. Open ChemDraw by clicking on the green hexagonal icon in the dock at the bottom of the screen. A blank document and accompanying Main Tools Palette will appear.
2. Click on: **File**  $\rightarrow$  **Apply Document Settings from**  $\rightarrow$  **ACS Document 1996**  
Followed by: **Object**  $\rightarrow$  **Fixed Lengths (should have a check mark)**  
Followed by: **Object**  $\rightarrow$  **Fixed Angles (should have a check mark)**

These settings will ensure proper sizing and structural consistency in the document.

3. Click on: **File**  $\rightarrow$  **Save As...** and save the new empty file to an appropriate location such as your space on the Novell file server. For instructions on using Novell, consult the Information Technology Web site at <http://www.wooster.edu/technology/documentation>.

Files should be named intuitively and systematically. Save the file for this exercise as *XYZ-CD-Tutorial.cdx* (in which XYZ is your initials). Ensure that the **Format** line at the bottom of the Save popup window is set to "CS ChemDraw Drawing."

## DRAWING BASICS: CREATING THE BENZYL CATION



4. The Main Tools Palette is used to create, edit, and move objects in ChemDraw. Begin by clicking on the Benzene Ring tool and then clicking anywhere in the document window. A benzene ring should appear.

5. If necessary, zoom in on the structure by clicking

**View → Magnify**

or zoom out by clicking

**View → Reduce**

6. HELPFUL HINT: Any errors in drawing can be corrected either with the Eraser Tool or by clicking

**Edit → Undo**

7. Create the external C–C single bond by first selecting the Solid Bond Tool on the Main Tools Palette. Move the mouse to the carbon vertex to receive the bond (a light blue highlight box should appear) and click the mouse.

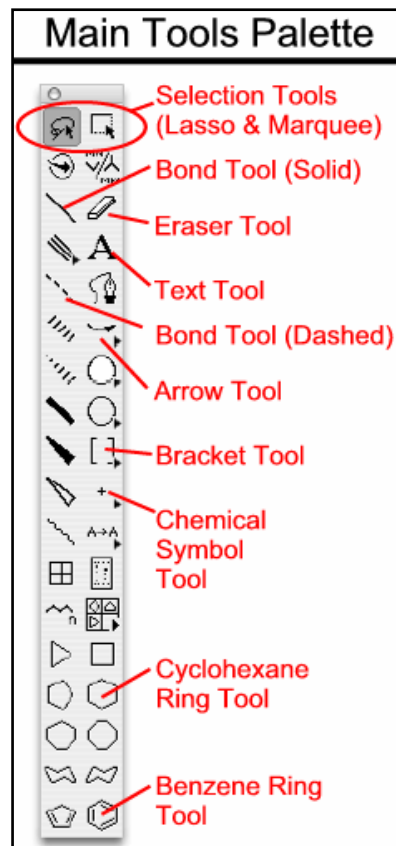
8. Draw the C–H bonds in a two-step process. First, draw two single bonds with the Bond Tool as in Step 4. Second, add “H” atom labels by either:

(a) moving the mouse over the end of the bond (a light blue highlight box will appear) and pressing “H” on the keyboard

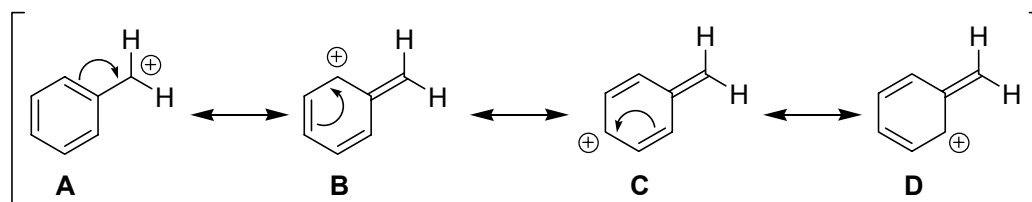
OR

(b) selecting the Text Tool, clicking on the end of the bond, and typing “H” in the resulting text box.


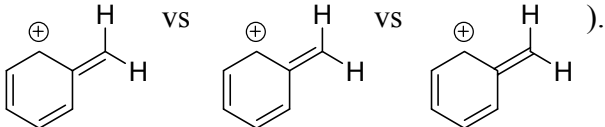
9. Click and hold on the Chemical Symbol Tool and select the positive charge from the popup menu. Click on the chemical structure to add a positive charge to the appropriate carbon atom. Congratulations! You have successfully completed your first structure.



## TAKE IT TO THE NEXT LEVEL: ARROWS AND RESONANCE STRUCTURES



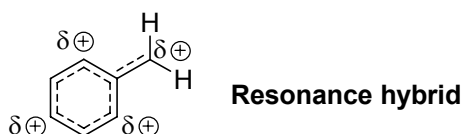
**Resonance contributors**

- Select the appropriate resonance arrow  $\longleftrightarrow$  from the Arrow Tool button. Drag the mouse in the main window to control the position, length, and orientation of the arrow.
- Objects can be moved** by highlighting with the Selection Tool (draw an outline with the marquee or lasso tool) and dragging them to a new location. The arrow keys on the keyboard can also be used to fine-tune the position of an object.
- Select the 120° arrow  from the Arrow Tool button. Click and hold the mouse button in the main window to define the beginning of the electron-pushing arrow. Drag the mouse to change the length and orientation of the arrow so that the arrow points from a pi bond towards the positive charge. After finishing, you may have to select and move the arrow to optimize its position.
- The second resonance contributor could be created by re-drawing the entire structure, but it is usually easier to copy, paste, and modify the original structure. Highlight the original resonance structure with either of the Selection Tools and click on:  
**Edit → Copy** followed by **Edit → Paste**
- Drag the pasted structure into position at the right of the resonance arrow.
- Modify the second resonance structure by erasing the electron-pushing arrow with the Eraser Tool, reducing the upper-right double bond to a single bond with the Eraser Tool, and moving the positive charge to the proper carbon atom
- Select the Bond Tool. Add a new double bond by moving the mouse over the center of the single bond (a light blue highlight box will appear) and clicking. Alternatively, the double bond can be constructed by dragging the mouse from one atom to the other. Clicking on the double bond will cycle through three different “looks” for the double bond (i.e.,  ).

- Complete the structure by drawing a new electron-pushing arrow.

18. Draw the remaining two resonance structures.
19. Click on the Bracket Tool and select square brackets []. Drag the mouse in the main window to place the brackets around the entire set of resonance structures.
20. Label the first resonance structure by clicking on the Text Tool and then clicking in the main window. Type the letter "A" into the text box that appears. Add the labels "B," "C," and "D" to the remaining resonance structures. Note that font type, size, and style can be changed, although the default font (10-point Helvetica) is typically sufficient.

### ALMOST THERE: DRAWING A RESONANCE HYBRID



21. Draw the backbone of the resonance hybrid with the Cyclohexane Tool. Add the partial pi bonds with the Dashed Bond Tool. Add the delta portion of the partial positive charges with the Text Tool. The Greek delta ( $\delta$ ) can be created by either changing a lower-case "d" to Symbol font or by pressing the OPTION and "D" keys simultaneously.
22. SAVE THE DOCUMENT.

### MECHANICS: TRANSFERRING FROM CHEMDRAW TO MICROSOFT WORD

#### 23. Within a Macintosh Platform:

- (a) Select the object(s) to be transferred with one of the Selection Tools.
- (b) Click on: **Edit** → **Copy**
- (c) In Microsoft Word, place the cursor at the desired insertion point and click on:  
**Edit** → **Paste**
- (d) The graphic should be inserted into the Word document. It can be repositioned and resized, although the "ACS Document 1996" default settings are usually fine.
- (e) To modify an inserted ChemDraw object, highlight the graphic in Word and paste it back into ChemDraw. Edit the object and then re-paste into Word.

**24. From a Macintosh to PC Platform:**

- (a) Verify that the document is saved in ChemDraw format.
- (b) Begin the process of saving the document as a TIFF image file by clicking:  
**File** → **Save as...**  
Change the parameter “Format:” at the center bottom of the dialog box from “CS ChemDraw Drawing” to “TIFF” using the scroll-down menu.
- (c) Name the TIFF file and note the location to which it is saved.
- (d) In Word, insert the graphic file by selecting: **Insert** → **Picture** → **From File...** and navigating to the TIFF file that you just saved.
- (e) Note that TIFF files cannot be edited; any modifications to the drawing must be done from the original ChemDraw document.

25. Congratulations! Feel free to explore the online tutorials and advanced features of ChemDraw. For additional practice, try to re-create a drawing from the textbook.

**26. Because there are a limited number of site licenses, be sure to quit the program when you are finished so that access is not blocked to other users.**

**TIPS FOR SUCCESS**

- Create the ChemDraw files well in advance of completing the lab report. Fortune rarely rewards those who wait until the last minute...
- Strive for consistency in
  - font type and size
  - bond lengths and angles
  - chemical notation (single vs. double-headed electron pushing arrows, resonance vs. equilibrium, etc.)
- Observe good layout practices by aligning objects logically
- Avoid producing an exact carbon-copy of graphics in the lab handouts.