

Chem 267. Tutorial on the Use of ChemDraw.

On the CRC computer, double click on the Macintosh HD icon. Double click on the Applications folder and look for the CS ChemOffice 2010 folder. Double click on the CS ChemDraw Pro icon. (Alternatively, if the ChemDraw icon is present in the dock, you may simply select that.)

To insert structures or reactions into another document such as Word, select the structures or reactions as described below, then copy and paste into the document.

(1) The Basics.

On the left is a tool palette. This is where you choose various tools for drawing structures.

Select the single bond tool (straight line) and click in the main window. A bond will be drawn. This is actually a line representation of ethane, $\text{CH}_3\text{-CH}_3$. Click on one end of the bond. A second bond forms. This would be propane, $\text{CH}_3\text{-CH}_2\text{-CH}_3$. Next click on the end of a bond and instead of letting the mouse button go, drag the mouse around. This will add another carbon but it allows you to place it at a different angle. Letting it add the carbon by itself produces a “normal-looking” structure.

Select the six-membered ring (cyclohexane) and click in the main window. A cyclohexane line drawing is produced. You can select the single bond tool and connect a CH_3 to one of the carbons of cyclohexane to make methylcyclohexane.

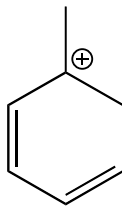
Selecting and moving objects. Select the lasso or marquee tool and click on a molecule. One click selects an atom or bond and double clicking selects the entire molecule. Several molecules and objects may be selected by surrounding the objects with one of the selection tools. The selection may be moved around by dragging it with the mouse.

To make a double bond, you can select the bond you would like to convert to a double bond, and by clicking on it with the single bond tool, it will change it into a double bond. If you would like to change it back to a single bond, you may use the eraser tool to do so. Just select the eraser tool and click on the atom or bond that you wish to erase.

To add a functional group, for example, OH, select the text tool and click on the atom that you want to change to that group. Type in OH and an alcohol will be drawn.

(2) Drawing Resonance Structures.

Draw the following molecule. To add the + charge, hold down the mouse button on the chemical symbols tool and select the circled + charge and point it at the atom to which you wish to place the charge.



If you click on the arrow box, you can find various types of arrows (i.e. equilibrium, resonance, reaction, and curved arrows). Choose the resonance arrow and draw two resonance structures for the molecule above. For this exercise as well, use the curved arrow tool to show the movement of electrons, and include brackets around the resonance structure using the bracket tool to indicate again that it is a resonance structure that is being drawn.

Copy and paste your resonance structures into your report.

(3) Drawing Reactions.

Draw 2-propanol. Next choose the reaction arrow from the tool palette and click next to the 2-propanol that was drawn. You can change the size of the reaction arrow by using the lasso tool or the marquee tool. Remember that if you would like to move whole molecules or multiple objects, select the lasso or marquee tool, select the desired objects, and drag around the highlighted content using the mouse.

Over the reaction arrow, use the text tool to indicate what reagents were used. For this reaction, above the reaction arrow indicate that concentrated sulfuric acid was used as a catalyst, and below the reaction arrow that heat was also used. For the products, draw propene ($\text{CH}_3\text{CH}=\text{CH}_2$) and water.

Copy and paste the reaction into your report.

(4) Exercises. Copy and paste these into your report.

Draw a molecule having 2 rings, 2 different functional groups, and 1 $\text{C}=\text{C}$ bond.

Look up the structure of the nucleotide guanine and draw it's structure.

Things you will need to know for the future that you should do on your own. These will not be included in your write-up. Eventually you will need to know how to draw stereochemical representations and reaction mechanisms.

Look up the structure of Vitamin D (there are various types) and draw one of its structures. Make sure to indicate the stereochemistry of certain bonds, using the wedge and dotted bond tools.

Choose a reaction from your lecture or lab text and draw the mechanism of the reaction. Be sure to draw curved arrows showing the movement of electrons and include any relevant reagents, conditions, or resonance structures needed for the reaction.

There is much that can be done with ChemDraw but you now know the basics. Play around with the different tools to become familiar with them. Some may make little sense but don't worry about those and don't try to learn everything at once.

-written by Matthew Liu, Chemistry, '11 and Peter Samal

(11/12/09 revision)