Fall 2023

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Lab Time: 1:15 pm – 5:15 pm T & Th, Discovery W408
Instructor office hours: By appointment.
T.A. office hour

This course will address each of the following departmental learning goals for chemistry majors:

1. Students will demonstrate general kn

results (i.e. why does the spectral data support (or not) the structure of the compound you are trying to make). A detailed experimental procedure and compo

Timeline of Laboratory Experiments

Day	Date	Title	Report Due
Thur	Aug. 31	NMR Training	
Tue	Sep. 5	2.1 Synthesis of a PET Molecular Sensor	Sept. 14
Thur	Sep. 7	2.2/2.3 Purification of a PET Molecular Sensor & pH Sensing	
Tue	Sep. 12	1.1 Green "Click" Chemistry	Sept. 21
Thur	Sep. 14	1.2 Olefin Metathesis in Micelles	
Tue	Sep. 19		

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Amended by Jordan Tocher and Matthias Brewer

The Chemistry Department at the University of Vermont is in possession of a site-license for ChemDraw. To download and install chemdraw please follow the instructions in the attached PDF: ChemDraw/ChemOffice Institution License – Quick start guide

As you read through the instructions and advice below you may

ChemDraw displays chemical structures in the "line-bond" form. That is, bonds are shown as black lines and carbons are represented by kinks in that line. Hydrogen's are implicit; there is assumed to be as many hydrogen atoms around each carbon as necessary to fill the carbon's octet. So, propane ($CH_3CH_2CH_3$) becomes:

The next section contains some sample compounds that you should attempt to draw in order to practice using the ChemDraw software.

Before embarking

are for all intents and purposes the same. However, the second scheme simply lists the reagents and lets chemists infer that the protonation step happens during workup, while the first scheme lists all the steps explicitly. Both methods are acceptable in the literature, but the second scheme helps you keep track of what's happening a little better, and <u>for the purposes of this class you should include the second step.</u>

Note also that when more than one step is shown for a reaction that occurs in the same pot, then both steps are numbered independently as (i) and (ii) and all the reagents and conditions for each step are grouped together. If two sequential but independent steps are being shown (i.e. you run a reaction, isolate the product, and then run a second reaction), then the individual steps are labeled (1) and (2) rather than (i) and (ii).

Please follow the following simple rules to keep your reaction schemes neat and clear:

(1)   Use the thinnest arrows from the ChemDraw drop-down menu.

(2)   Provide reagents above the reaction arrows and reaction conditions below the reaction arrows.

(3)   If available, provide the reaction yields below the reaction arrows.

(4)   Number your compounds with bold numbers/letters below the structures.

(5)   Keep things aligned! Clicking on "*View*" -> "*Show Crosshair*" can help a lot with this endeavor. For challenging alignment/distribution tasks, select the objects you need to align/distribute and click on "*Object*" -> "*Align*" or "*Distribute*". The distribute function holds the outermost structures fixed and then distributes the rest of the structures evenly spaced between them.

        : When drawing several similar structures, it is usually easiest to copy and paste a structure and then modify it, rather than re-drawing the whole thing from scratch. To copy a structure and keep it aligned with the original:

                a) Select the structure to be copied (with the Lasso or Marque)

                b) Press and hold down the control and shift keys and also the left mouse button while dragging the structure to be copied either straight up/down, or left/right.

(6)   Only use a solid reaction arrow if the reaction is confirmed to work. For proposed or ongoing reactions use a dashed reaction arrow.

(7)   Minimize the white space in your reaction schemes.

(8)   Keep all reaction arrows either horizontal or vertical, avoiding diagonal arrows.

ChemDraw contains a variety of curved arrows to use for drawing arrow-pushing mechanism. Sometimes getting things aligned just right is a bit tricky, but you can usually muddle through just fine. If a more elegant solution is needed, curved arrows can be drawn with the "*pen*" tool, which can draw more sophisticated Bezier curves. You can add an arrow to either the end or start of any Bezier curve by simply right clicking onto the curve and selecting "Full/Half Arrow at Start/End". Also note that you can readily adjust the shapes of your Bezier curves at a later point in time. To do so you have to, however, first select the curve and then click on the "*pen*" tool again. More detailed instructions on how to draw stunning mechanistic arrows in ChemDraw can be found online at:

http://www.chemistry-blog.com/2011/12/09/neat-o-curved-arrows-in-chemdraw/

Overall, this document is intended to be a rudimentary beginners guide which will allow you to install the ChemDraw software on your computer using the UVM site license, and teach you some of the tools within the software. Organic chemistry has a lot of conventions associated with how molecules are drawn, but these well-established rules provide clarity in communications. With a little practice, you will be correctly drawing beautiful molecules in no time!

As with anything CHEM 047 related, never hesitate to ask me for help, especially when you are first starting to use the software!