

UMass Amherst has a site license for ChemDraw (the academic and industrial standard for generating chemical structures), which means you can download a copy for personal use, free of charge. Your first assignment will be to become familiar with ChemDraw. This is non-optional and is worth 50 points. To download the software, see the document “Detailed Software Download Instructions” just below the link to this handout on the course website.

Then . . .

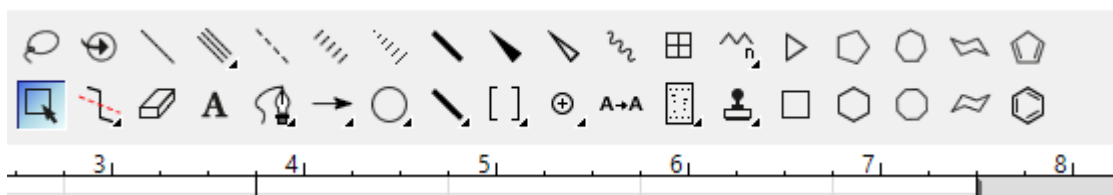
Download the ELN non-formal template on the homepage and get started!

This activity is so you can become familiar with ChemDraw and Gradescope, the website we will use to grade your pdf reports electronically, and to earn an easy 50 points. Do all exercises below. **Upload your report to Gradescope by 11:59 pm on the Wednesday of week 1.**

(1) Open ChemDraw. Click the File menu, highlight open style sheets, and choose “ACS document 1996.” This will have all text, bond lengths/angles, etc. preformatted for you and it is this formatting that is to be used for all ChemDraw made structures.

The Main toolbar (Figure 1) should be there upon opening, but if it is not, click view at the top of the menu options, and then check “Show Main Toolbar.”

Figure 1. The main toolbar in ChemDraw.



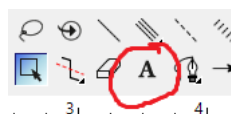
Make sure the style toolbar (Figure 2) is also there. Follow the above steps and check “show style toolbar.”

Figure 2. The style toolbar in ChemDraw.



Let's start simple. On the main toolbar, click the “A”. This is the text function. Type the molecular formula of caffeine ($C_8H_{10}N_4O_2$), but do not add subscripts.

Figure 3. The text function



When you are finished typing the formula, click the select button. See Figure 4.

Figure 4. The select function.



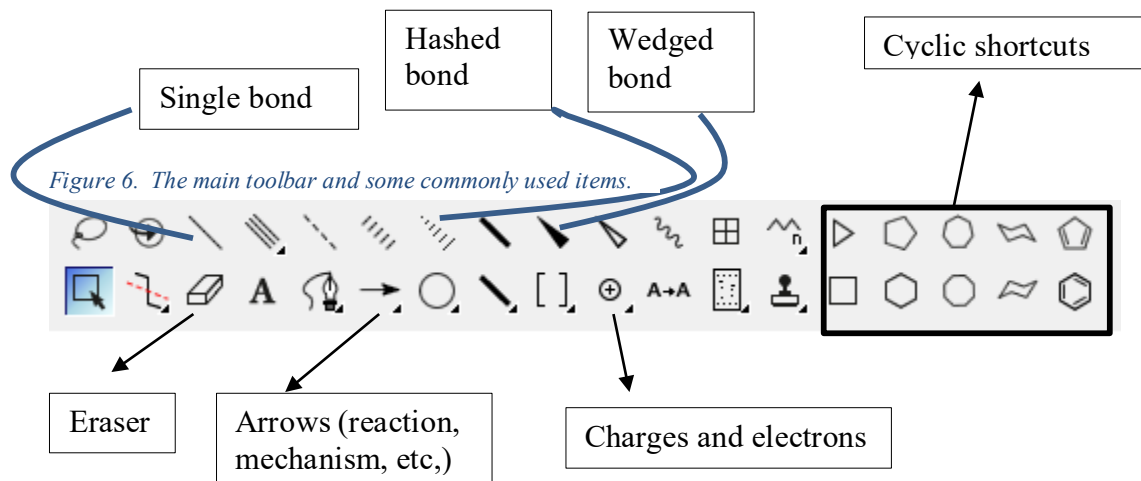
When your text is selected, click the formula button on the style toolbar. See Figure 5.

Figure 5. The formula button.



Notice how all element numbers automatically change to subscripts. The same will happen with charges! Do not copy and paste ONLY TEXT from ChemDraw to Word. The formatting (sub- and superscripts, etc) will not be preserved.

(1A) There are no activities in this section. Just information on the main toolbar. Figure 6 shows the main toolbar and what some of the most common buttons do. If you forget, simply hover over the button and it will tell you what it is for.



- On some of the buttons you should notice a little black arrow. This means other related items appear under this button. To get to these other items, click and hold the button and then drag to the desired function.

The next section is where the report will start.

(2) This section will guide you in drawing *trans*-3-bromocyclohexanol.

- On the main toolbar (MT), click the cyclohexane shortcut, then click in the workspace. ChemDraw will insert cyclohexane. Do not modify the formatting.
- Again on the MT, click the wedged bond (Figure 6).

- Hover cursor over any one of the carbon atoms (notice the light blue ball ChemDraw uses to recognize where you want to manipulate). Click the mouse. ChemDraw will insert a wedged bond (right now a methyl group)
- Hover over the end of the wedged bond. On your keyboard, simply press the “B” key. ChemDraw will insert a bromine atom.
- This shortcut works for many common atoms that organic chemists use (S is sulfur, C is carbon, P is phosphorous, etc.). If you need a different atom, click view, then choose periodic table window. Click the atom needed, then click at the end of a bond. ChemDraw will insert that atom. You should now have bromocyclohexane.
- On the MT, click the hashed bond (see Figure 6). Go to the third carbon on the ring (doesn’t matter the direction you go around the ring).
- Hover the cursor over the carbon atom and click. You now have drawn trans-3-bromomethylcyclohexane, but we need to turn that methyl group into an alcohol.
- Again, hover over the end of the hashed bond and press the letter “O” on your keyboard.
 - Notice how ChemDraw not only automatically inserts an oxygen atom, but its corresponding hydrogen as well. It does this because oxygen must be bound to two things to be neutral.
- Now we need to copy and paste this structure into your Electronic Lab Notebook (ELN), which is a MS Word non-formal template (downloadable on the course website). First, save the template so you always have it available offline. Then:
 - Delete all sections (not the headings, name, TAs name, exp. name, etc).
 - Call the first section trans-3-bromocyclohexanol.
 - In ChemDraw, select your entire structure.
 - Right-click (or the Mac equivalent) and select copy.
 - In the ELN, put the cursor just below the first section. Right-click again (or the Mac equivalent) and select paste.
 - Double click on the structure. ChemDraw opens and this structure is editable within the Word document. Close the ChemDraw window (small ‘x’) and Word is now the active document.
 - If this does not happen on your computer, it is ok! This is merely a convenience, not a requirement.

The next section is unguided. If you do not know the structure of the name provided, look it up. Here, Wikipedia is very useful.

(3) Draw the molecules below in ChemDraw. Each molecule/ion must have its own section in your ELN with an appropriate heading.

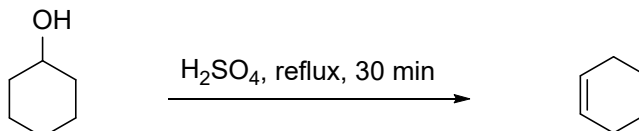
- (2R)-2-butanol (must be this enantiomer).
- Benzoic acid
- Sodium benzoate (conjugate base of benzoic acid), showing all lone pairs of electrons and the position of the formal charges.
- cis*-1-*tert*-butyl-4-methylcyclohexane (do not draw a chair structure unless you are very comfortable with *cis/trans* in a chair).
- Caffeine (look up the structure).

The next section has you practice drawing a reaction scheme.

(4) Reaction Schemes

A reaction scheme shows only the overall reaction (starting material, reagents, conditions and product(s)) all in one scheme. DO NOT SEPARATE MULTI-STEP PROCESSES OR SHOW ENTIRE MECHANISMS.

- Recreate the reaction scheme below in ChemDraw.



For the reaction arrow:

- Click the arrow on the MT (see Figure 6).
- Click the mouse. ChemDraw will insert a straight reaction arrow of a default length.
- Notice the layout, formatting, etc. The reaction conditions, reagents, etc. should NEVER be longer than the arrow.
- If the reaction arrow needs lengthening, select it and then adjust using the corners of the now highlighted arrow.

For the alkene:

- Click the single bond tool (Figure 6).
- Hover over a carbon-carbon bond and click.
- ChemDraw will insert a pi-bond automatically.

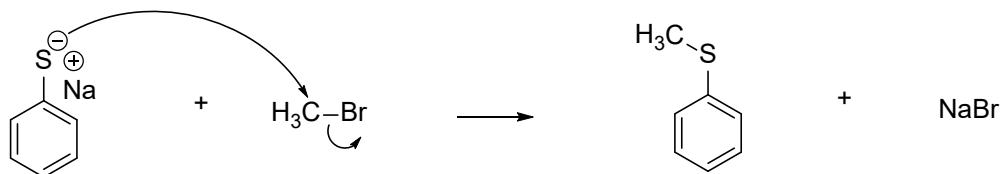
Copy and paste into your ELN ChemDraw report (must be in its own section, properly headed).

The next section has you practice drawing a reaction mechanism.

(5) Reaction Mechanisms

A mechanism shows the flow of electrons, represented by curvy arrows, as a reaction proceeds. This shows exclusively which bonds are forming and breaking. Recreate the mechanism below.

- The mechanism, curvy arrows are a sub-tool in the arrow button on the MT (Figure 6). Click and hold, then drag to the appropriate curvy arrow, then release the mouse button. This arrow is now selected and the icon on the MT will change to it. Be careful, some are half-headed for single electron radical mechanisms!



- Once you have the curvy arrow selected, click and hold, then drag to the appropriate atom.
 - Curvy arrow angles are fixed. Sometimes the angles are way off. To temporarily disable the fixed angle, click and hold as above and then press and hold the Alt key. This will allow you to point the arrowhead exactly where it needs to go.

Copy and paste into your ELN ChemDraw report (must be in its own section, properly headed).

Next, you need to convert your Word file to a pdf. You can save as, or print as a pdf so you can upload to Gradescope.

Upload your report to Gradescope by 11:59 pm on the Wednesday of week 1. To do this, follow the steps below:

1. Log in to your UMass email.
2. In the email from Gradescope, follow the instructions to set your password.
3. Once logged in to Gradescope, click “Chem-269”
4. Click on ChemDraw Lab assignment
 - a. For future labs, click on the appropriate name of each experiment.
5. On the next window, click “submit pdf”
6. On the next window, click “select pdf”
7. Navigate to your document, double click, then click “upload pdf”
 - You will have to tell Gradescope on what page(s) each question/topic is. Click the question/topic on the left side, then click which page it is on by simply clicking on your documents page. If your question/topic extends to two different pages, click the first page it’s on, then the next and so on.
8. At the very bottom, and to the right edge of the screen that follows, click “submit”

Important: Make sure you read on to the next page.

You will become more familiar with other options as you get further into the semester. Please feel free to ask Dr. McDaniel (ISB 241F) or your TA questions about ChemDraw if the need should arise.

When you are finished with this ChemDraw activity, go to the course website and navigate to the Schedule of experiments> Check-In and Melting Point Experiment> First Day Handout - Start Here