



ChemDraw User Guide

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The following is a guide to creating accurate ChemDraw figures for papers, presentations, and posters. This is by no means a comprehensive guide; however, these instructions will help you make the best figures possible. Please ask Professor Ball if you have any questions or suggestions.

ChemDraw is a tool that scientists use to depict chemical structures, reaction schemes, mechanisms, tables, and figures. What you draw in the program is meant to be a pictorial depiction of the structure and reactivity of your molecules. You can download this program here:

<http://sitelicense.cambridgesoft.com/sitelicense.cfm?sid=124>. Use your Amherst e-mail for access. It will not work with a non amherst.edu address

1.1 Settings

For most publications and any presentation, the standard setting is "ACS Document 1996".

- 1) Open a new document
- 2) Go to "File", "Apply Document Settings from", and choose "ACS Document 1996" from the list.
- 3) Go to "view" and make sure the following are checked: gridlines, general toolbar, style toolbar and general warnings. These settings will help you align your structure, present tools to draw your structures, and produce warnings if you are exceeding the valency of the atom (depicted by a red square on you structure).
- 4) It is important to start with set bond length and angles. This will prevent the drawing of bond angles that are not appropriate for the atom. The program will automatically draw the angles and appropriate bond lengths. Go to "Object" and make sure "fixed length" and "fixed angles" are both checked.

1.2 Copy and paste

In general for one project you should use the same document. You can expand the size of your ChemDraw workspace by changing the document size under "File", "Document Settings". **SAVE FREQUENTLY!!!**

- For papers: Please read the parameters outlined by the journal.
- For PowerPoint presentation: Copy, and resize to 120%.

- For Word: Word will resize your drawing based on its dimensions. In general between 60% - 80% resizing is appropriate. Make sure all your structures are the same size.
- For posters: Copy and resize to at least 120%, this will depend on the format of your poster.
- You should be able to copy and paste back and forth between any Microsoft Office document and ChemDraw. This called “round trip editing”.
- NOTE: for Mac users who have Microsoft Office 2010 or afterwards, there is a file you need to download an update to Office (14.0.1) to do round trip editing. See the link below to find out how. <http://forums.cambridgesoft.com/messageview.aspx?catid=42&threadid=1915>

Now you are set! Below are basic tips and instructions on drawing structures salient to CHEM 231 and other classes.

2.1 Drawing Bond Angles

Remembering from introductory general and organic chemistry courses, each element when making bonds has a distinct electron configuration and orbital angles (e.g. VESPR theory). For example, carbon has four valence electrons that are sp^3 , sp^2 , or sp hybridized. These considerations are built into ChemDraw. For instance, when you draw butane ($CH_3CH_2CH_2CH_3$) each carbon should be sp^3 hybridized with the bond angles of 109° . You can try to do this manually, but ChemDraw can do this for you. On the left, there is a “Tools” toolbar. Click on the multiple bond icon on the bottom left of the toolbar and in the pop-up box choose the straight chain icon on the left. Drag your cursor along the screen until you have four carbons. The program will give you a number as you drag to tell you how many carbons are present. What you notice is that ChemDraw has made four carbons with the appropriate 109° angles. ChemDraw assumes hydrogens in its drawings. Therefore, at each intersection of two bonds in butane, two hydrogens (CH_2) are implied and at the 1st and 4th carbons three hydrogens are implied (CH_3).

2.2 Multiple bonds

What if I wanted to make double or triple bonds? Let's draw 1-butene where a double bond is between the first and second carbons. Draw butane as described before. You can draw the double bond two ways: 1) click on the single bond icon and simply draw another single bond over the existing one between the 1st and 2nd carbons or 2) go the “tool” box and click on the multiple bond icon and choose the double bond and drag it over the existing single bond. For a triple bond, just repeat the action.

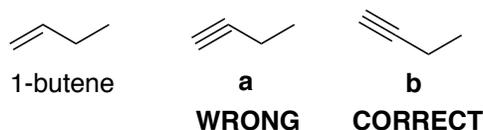


Figure 1. Drawing multiple bonds.

- Note: Triple bonds are hybridized so that they are at a 180° angle. So your triple bond for 1-butyne should like Figure 1b not 1

2.3 Cyclic compounds

You can draw these yourself; however, ChemDraw has several templates for 3, 4, 5, 6, and 7-membered rings. They are at the bottom on the tools bar. Please use them! They will draw your rings at the appropriate lengths and angles according to your document settings. To make bicyclic molecules like indole, first draw the aromatic ring with the benzene icon. Next, choose the five-membered ring icon hold and click on the first carbon where the cycles will meet and drag to the second. Click on the carbon you want to change to nitrogen (you should see a small filled square) and type "NH". Next draw the appropriate double bond by choosing the bond tool and simply clicking once on a single bond (Figure 2).

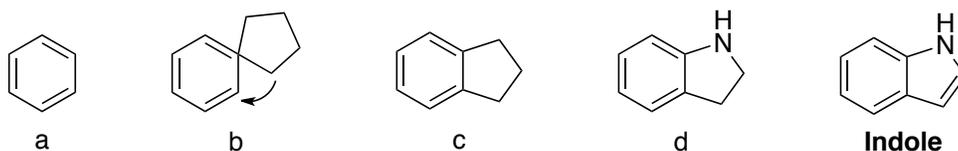


Figure 2. Steps to drawing bicyclic compound indole. a) draw benzene, b) use the 5-member ring tool and click on one carbon, c) drag to second carbon, d) add text, then double bond.

2.4 Amino Acids and Stereochemistry

Most amino acids are chiral molecules and have absolute stereochemistry. For example, if you draw methionine like in Figure 3a, it is very ambiguous if it is D- or L-methionine. Therefore, it is important that you use the "wedge" tool in the tools box to denote the stereochemistry when you are using a specific isomer. Solid wedge means your bond is coming out of the screen and the hollow wedge means the bond is going behind the screen. Typically the R-group of the amino acid is the one that is denoted in stereochemistry. Most amino acids have (S) stereochemistry at the alpha carbon, except cysteine (R) and glycine, which is achiral. See this link from wikipedia for a list of L-amino acids with the correct stereochemistry

(http://en.wikipedia.org/wiki/File:Amino_Acids.svg). Note that the R-groups are with solid wedges indicating that they are coming out of the plane. If you are not sure if you have drawn the appropriate isomer, refer to an organic chemistry text book to learn how to determine if is a (S)- or (R)- isomer.

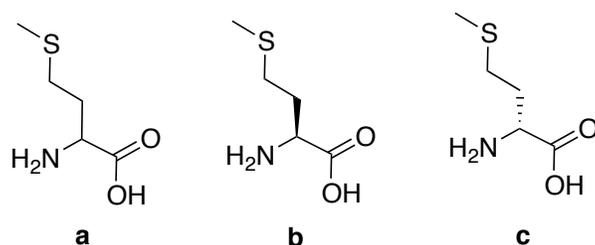


Figure 3. Depictions of methionine: a) racemic, b) L- or (S)-Methionine, and c) D- or (R)- Methionine

2.5 Inorganic Compounds

Drawing inorganic/organometallic complexes can be a quite a challenge. This is because unlike organic molecules that are drawn with linear (sp), bent (sp^2), or tetrahedral (sp^3) geometries, inorganic/organometallic complexes have an expanded range of geometries. Adding complex ligands to these metal centers require significant manipulations of bond lengths to allow clear depiction of the metal center. Start by drawing the inorganic complex with a fixed bond length and angles and change things accordingly after they are drawn (Figure 4).

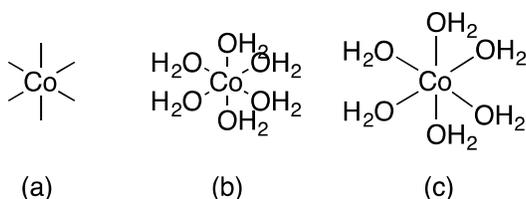


Figure 4. Steps to drawing an inorganic complex (a) Draw metal center then bonds, (b) draw the ligands, (c) elongate bonds and align atoms.

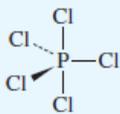
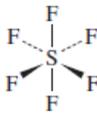
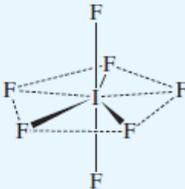
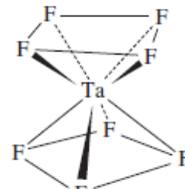
| Steric Number | Geometry | Examples | Calculated Bond Angles | |
|---------------|------------------------|-----------------------------------|------------------------|---|
| 2 | Linear | CO ₂ | 180° | O=C=O |
| 3 | Trigonal (triangular) | SO ₃ | 120° |  |
| 4 | Tetrahedral | CH ₄ | 109.5° |  |
| 5 | Trigonal bipyramidal | PCl ₅ | 120°, 90° |  |
| 6 | Octahedral | SF ₆ | 90° |  |
| 7 | Pentagonal bipyramidal | IF ₇ | 72°, 90° |  |
| 8 | Square antiprismatic | [TaF ₈] ³⁻ | 70.5°, 99.6°, 109.5° |  |

Figure 5: Geometries of coordination complexes according to steric number (Miessler and Tarr, 5th Ed.)

2.51 Trigonal complexes

Trigonal complexes are tricoordinate complexes and ligands align along an x,y plane. Bonds angles are ideally 120°.

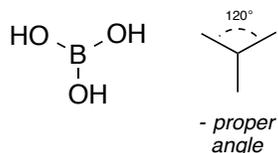


Figure 6: Drawing and ideal angles of B(OH)₃ a trigonal complex.

2.52 Square Planar complexes

Square planar metal complexes are tetracoordinate and ligands are aligned along a x,y plane. In many inorganic textbooks wedges are used to indicate this planar orientation (Figure 7a). You may choose whichever representation, just stick to it! Square planar metal complexes are often depicted in the plane of the screen (Figure 7b) or drawn to show a 3D perspective (Figure 7c). The ligands lie on an x,y plane at an ideal 90° (*cis*) and 180° (*trans*) from each other. The ligands on your molecules may require slight perturbations from the ideal angles.

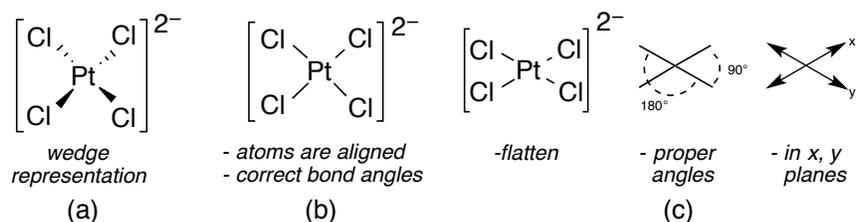


Figure 7. Different representations of a $[\text{PtCl}_4]^{2-}$

3.1 Drawing Reaction Schemes

There are three basic rules in drawing a reactions scheme:

- 1) Starting materials are on the left, products are on the right
- 2) Reagents, solvents, temperatures and reaction times are over the arrow. In general, each step in the reaction is numbered. What constitutes a step? Every time you have an isolation step, add another reagent after a period of time, or change solvent it is a step. There are exceptions. If unsure, please ask an experienced group member.
- 3) In a synthesis, you should note your yield. Use only two significant figures.

Important tools in making great reaction schemes are the alignment tools under the **objects** menu. The two major tools are **align** and **distribute**. “Align” allows you to properly line up your structures, text, symbols, and reaction arrows. “Distribute” allows you to space out the structures evenly.

In figure 8, a reaction scheme to make a Se_2BS_3 crosslinker is depicted. The starting material is on the left and product is on the right. All structures, text, and arrows are aligned. Reaction time, and temperature are listed. Note, Sulfo-NHS is an uncommon chemical. Its structure is drawn out and labeled.

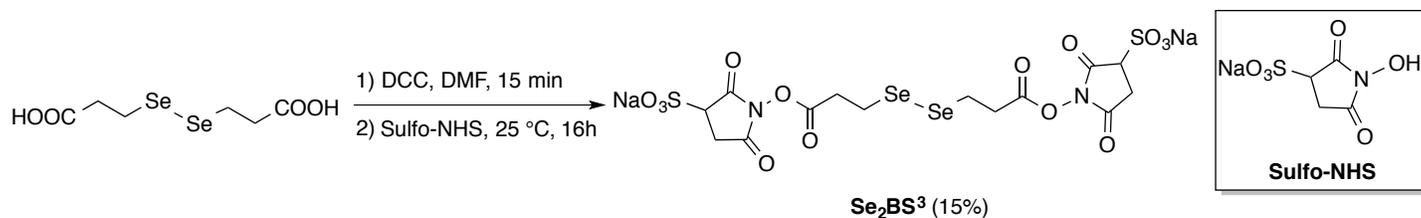


Figure 8. A sample reaction scheme of the synthesis of a Se_2BS_3 crosslinker.

***Tips:** 1) Use the gridlines to align your structures, 2) Highlight the parts that should move together and group them (Ctrl + G for PC or ⌘G for Mac). Once grouped, highlight each segment and choose “object”, “distribute”, and “horizontally” to distribute along the x-axis or “vertically” along y-axis. Do the same to align the structures. “Align L/R centers” or “align T/B centers” are the most useful.

3.2 Reaction mechanisms

Drawing mechanisms is an exercise in arrow pushing. It demonstrates where the electrons are going and how they make and break bonds to form your desired product. The key to drawing a correct mechanism is to remember that the tail of the arrow denotes where the electrons originate (Figure 9). The head of your arrow points conveys where the electrons are going. Please keep this in mind or you will several break laws/principles of physics. **Remember your lone pairs and charges!** Notice the tetrahedral depiction of the alkoxide in Figure 9; this is a proper depiction of a sp^3 carbon. The use of a solid wedge unambiguously denotes a specific stereochemistry. **Challenge:** Does the alkoxide have *R* or *S* stereochemistry?

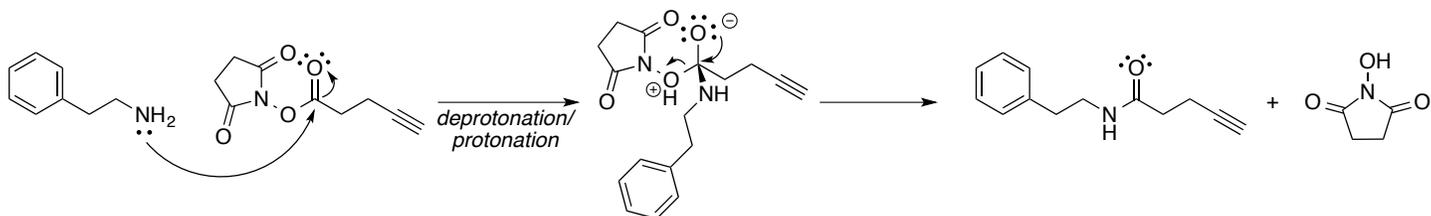


Figure 9. Mechanism of an amine coupling with an alkyne-NHS ester.

4. Conclusion

There are many other tricks and applications of ChemDraw that can help you make excellent schemes and figures. Feel free to explore the program and your CHEM 231 instructors and fellow class members! Additional tutorials and help can be found in ChemDraw by clicking on **Help** and selecting **Getting Started**. In Help, double click on **Getting Started** in the new window and choose **ChemBioDraw User Interface**. This will allow you to become more familiar with the different toolbars in the drawing workspace. When you feel confident you understand the set-up of ChemDraw, double-click on **Tutorials**. **Complete Tutorials 1, 2, and 7.**

Want to be a ChemDraw pro? Check out the amazing YouTube video below that will have you well on your way!

<http://www.youtube.com/watch?v=03WNbvZLDkk&fmt=22>