

Compound name	Molecular Weight (MW)	density (g/mL)	Volume (mL)	Weight (mg or g)	mMoles	Ratio
benzaldehyde						1
(carboxymethylene) triphenylphosphorane		---	---			
hexanes	---	---		---	---	---

2. Determine the amounts of each reagent that you will need if you were to scale the reaction to 5 mmols of benzaldehyde. (See Mohrig 27.2.) Write out a new reagent table.

Compound name	Molecular Weight (MW)	density (g/mL)	Volume (mL)	Weight (mg or g)	mMoles	Ratio
benzaldehyde					5	1
(carboxymethylene) triphenylphosphorane		---	---			
hexanes	---	---		---	---	---

3. Recommend glassware that you would need to complete the reaction at this scale. (See Mohrig 27.2)

III. ChemDraw Assignment

This assignment requires that you download and learn to use a program. You have plenty of time to finish this assignment, even if you have technical difficulties with the program, provided you start early!

ChemDraw is a program designed for drawing molecules and reactions. The software is easy to use, but the more time you spend exploring available options and practicing using the program, the easier it will be to properly complete your future lab reports. In this assignment, you will be asked to complete several tutorials, explore IU faculty web pages, draw a scheme from a future lab project, and answer some questions about the program. Combine all of this information into a Word (or other similar word processing program) document by the beginning of your lab period next week.

To complete this assignment, you must obtain a copy of ChemDraw. IU has purchased a site license for this software, so it is free for any IU student to download and use. Use the link below to download the program or use one of the computers in room 046 of the Chemistry Building. Keep in mind that your schemes for all of your lab reports for this class must be drawn in ChemDraw. I recommend saving your work in ChemDraw as you go along.

Download ChemDraw:

1. Connect to the link iuware.iu.edu
2. Select the "Analysis & Modeling" tab on the left hand side
3. Click on "ChemBioDraw 13" (or the most recent version)
4. Follow the directions to complete your download of ChemBioDraw 13 (you must use your IU e-mail address to be able to use the site license.).

Once you open ChemDraw:

The first thing that you should do is to create settings so that all of your structures are neat and consistent. **For purposes of this class, I would like all drawings to use the settings called "ACS Document 1996". To do this, go to "File" → "Apply Document Settings From..." → "ACS Document 1996".** Please do not make any changes to these settings, and use them for ALL subsequent reports.

Tutorials:

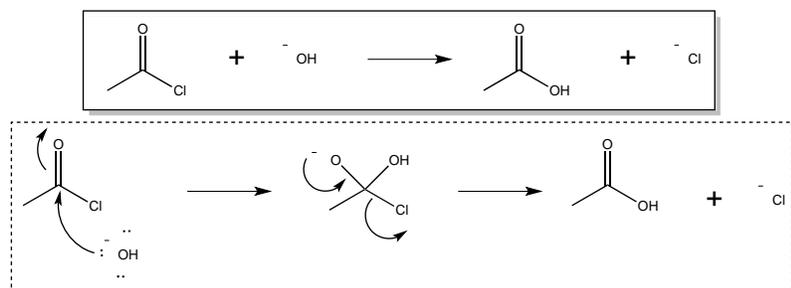
ChemDraw comes with several tutorials that provide step-by-step directions for using standard features of the program. You can find these tutorials by selecting the help menu and clicking on "Getting Started" from the menu. After completing each of the following tutorials, **Copy and paste each of the structures you drew into your assignment.**

Please complete the following tutorials:

Tutorial 2: Using Rings

Tutorial 6: Showing Stereochemistry

Now that you are an expert at drawing structures, it's time to figure out how to draw arrows (both reaction arrows and mechanistic arrows). There are more items in the help menu that you can refer to if necessary. **Draw the following reaction scheme and mechanism in ChemDraw with the correct formatting:** (If you do this correctly, your scheme will look much better than this one!)



IV. IU Chemistry Faculty Web Sites and Proper Referencing:

A wide variety of research takes place here at IU, and it's a good idea to know what this research is and how it relates to your class work. Therefore, I would like you to take some time looking at some of the research areas studied in the department by going to the research faculty web site:

<http://www.chem.indiana.edu/faculty-research/faclist.asp?t=Research>

The department is comprised of several divisions, and I would like you to focus on the research of faculty who list Organic chemistry as their primary discipline. There are six faculty members who fall into this category: Professors Aron, Brown, Cook, Pohl, VanNieuwenhze, and Williams. Visit each of their websites, and choose one natural product and one reaction scheme (total, not one from each). **Draw the natural product that you have selected in ChemDraw, being sure to correctly show any stereochemistry and making the structure as neat and professional looking as the drawings on the web sites. Again, transfer this drawing to your lab report. Do NOT cut and paste from the webpages!**

Insert a reference to the journal article where the natural product synthesis or reaction scheme was reported, and be sure to use correct ACS formatting (this will be graded). You can find the ACS Style Guide online at <http://pubs.acs.org/isbn/9780841239999>. It is an excellent resource for writing in this

class, and you can use it to learn about proper citation. In this class, we will use the format of *The Journal of Organic Chemistry*, which is superscript numbers.¹

V. Questions:

Answer each of the following:

1. *How can ChemDraw be used to predict the ¹H and ¹³C NMRs of acetophenone? (Include these NMRs in your lab report.)*
2. *How can you use ChemDraw to convert a structure into a name and to convert a name into a structure? What is the structure of (R)-4-(1-phenylpropyl)benzaldehyde?*
3. *How can ChemDraw calculate an exact mass to four decimal points past the zero and molecular formula? Paste the exact mass and molecular formula of (R)-4-(1-phenylpropyl)benzaldehyde in your assignment.*
4. *Define what the following shortcuts do:*
 - a. *Ctrl C*
 - b. *Ctrl Z*
 - c. *Ctrl V*
 - d. *Ctrl G*

Some Useful Notes:

1. All schemes and structures should be as neat and look as professional as possible.
2. Arrows should not touch bonds or atom labels.
3. Charge symbols should not overlap with atom labels.
4. All structures in all future lab reports must be drawn by the report author in ChemDraw.

¹ Coghill, A. M., Garson, L. R. *The ACS Style Guide: Effective Communication of Scientific Information*, 3rd ed.; American Chemical Society: Washington, DC, 2006; p287.