Chapter 6: Writing Lab Reports

During previous chemistry lab courses you took, you might not have been required to write lab reports. One goal of this course is to allow you to get familiar with the way lab work is recorded and presented to other people, and this includes writing full lab reports.

6.1 Choosing and Keeping a Laboratory Notebook

The laboratory notebook is an integral part of organic chemistry. Published scientific papers always include a detailed, accurate experimental record. In an industrial laboratory, the notebook may be used as a legal document when applying for patents. Potential scientists – whatever their field – must learn to keep a detailed account of their work. This allows someone else both to review the work and to repeat it exactly. Extrapolating to the student laboratory, if a particular experiment does not work well for you, the instructor will want to know why. Your detailed written procedure and observations can give clues to experimental failures. Therefore, the lab notebook is strongly emphasized in the organic chemistry lab courses.

You are required to use a laboratory notebook that produces a copy of your work. Several manufacturers produce bound carbonless laboratory notebooks (available at the University bookstore). The pages in these books are marked with a grid and numbered. A loose-leaf or spiral notebook is not acceptable because pages are easily removed and lost. Do not use loose pieces of paper for keeping laboratory records!

Write your name and laboratory section number on the cover of your notebook. Then, enter experiments consecutively in ink. Write the date on the top of the page. Every entry should be clearly legible, but impressive neatness is not required. If you make a mistake, do not erase them or rip out the page. Instead, draw an "X" over the section and go on.

6.2 Calculation of Theoretical Yield

The theoretical yield of a reaction is the amount of product that would be formed if the reaction went to completion. It is based on the stoichiometry of the reaction and ideal conditions in which starting material is completely consumed, undesired side reactions do not occur, the reverse reaction does not occur, and there are no losses in the work-up procedure.

In order to calculate the theoretical yield, you must first balance the reaction. Then, look closely to determine which reagents are being used in excess and which is the limiting reagent. The overall yield of product depends on the limiting reagent. Remember that catalysts, solvents, or any compounds that are not part of the actual chemical reaction cannot be the limiting reagent. Theoretical yield calculations are carried out in the same way as they were in general chemistry: the moles of limiting reactant determines the moles of product.

After your laboratory reaction is complete, you will isolate and measure the amount of product, then compare the actual yield to the theoretical yield to determine the percent yield using the equation shown below.

$$\frac{\text{actual yield}}{\text{theoretical yield}} \times 100\% = \text{percent yield}$$

It doesn't matter what units you use for actual and theoretical yield – grams, moles, milliliters, etc. – so long as both values are in the same units.

In the laboratory, the percent yield has the practical aspect of telling you how successful your synthesis scheme was. A low percent yield means that the conditions were not optimal and could be improved. Perhaps there are competing reactions occurring or some of the product is being lost in the purification steps.

To calculate theoretical yield:

1. Balance the reaction and determine the stoichiometry or ratios of reactants to products.
2. Find the number of moles of each starting material used.
3. Determine which reagent is limiting.
4. Calculate the moles of product expected if the yield were 100% based on the limiting reagent.
5. Calculate the grams of product corresponding to the number of moles expected.

Example Problem 1

What is the theoretical yield of ethylene in the acid-catalyzed production of ethylene from ethanol, if you start with 100 g of ethanol? If you perform this reaction and isolate 51.82 g of ethylene, what is the percent yield?

$$CH_3CH_2OH \xrightarrow{H^+} CH_2{=}CH_2 + H_2O$$

The reaction as written above is balanced, with one mole of ethanol producing one mole of ethylene, therefore the stoichiometry is 1:1. The acid, written over the arrow, is a catalyst and does not enter into the theoretical yield calculations. To calculate the theoretical yield, determine the number of moles of each reactant, in this case the sole reactant ethanol. Convert the 100 g to moles; the molecular weight of ethanol is 46 g/mole, therefore:

$$100 \text{ g x } \frac{1 \text{ mole}}{46 \text{ g}} = 2.17 \text{ mole}$$

Since there is only one reactant, it is also the limiting reagent. The theoretical number of moles of ethylene is 2.17. Since the molecular weight of ethylene is 28 g/mole, this corresponds to 61 g from the following calculation:

$$2.17 \text{ mole x } \frac{28 \text{ g}}{1 \text{ mole}} = 61 \text{ g}$$

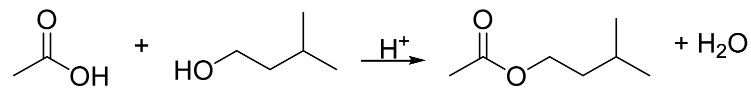
The theoretical yield is therefore "61 g." Note that theoretical yield is expressed as mass or "grams."

To calculate percent yield, divide actual by theoretical yield:

$$\frac{51.82 \text{ g}}{61 \text{ g}} \text{ x } 100\% = 85\%$$

Example Problem 2

Consider the acid-catalyzed esterification of isoamyl alcohol to produce isoamyl acetate. If you begin with 10 g of isoamyl alcohol, 5 mL of acetic acid, and 1 mL of sulfuric acid, what is the theoretical yield of isoamyl acetate? If you perform this reaction and isolate 3.21 g of isoamyl alcohol, what is the percent yield?



The reaction as written above is balanced, with one mole of acetic acid and one mole of isoamyl alcohol producing one mole of isoamyl acetate and one mole of water, therefore the stoichiometry is 1:1. The acid (sulfuric acid), written over the arrow, is a catalyst and does not enter into the theoretical yield calculations. Next, determine the number of moles of each reactant. To do this, look up the molecular weights and densities of the reactants and product (see Chapter 2 for where to find this information).

Compound	MW	Density or sp. gr.	Other information
Isoamyl alcohol (butanol, 1-, 3-methyl)	88.15	0.809	
Acetic acid	60.05	1.05	conc. reagent is 17.4 N, 99.8% by weight
Isoamyl acetate (acetic acid, 3-methylbutyl ester)	130.19	0.867	

10 g of isoamyl alcohol will produce 0.11 mole of isoamyl acetate:

$$10 \text{ g x } \frac{1 \text{ mole}}{88.15 \text{ g}} = 0.11 \text{ mole}$$

5 mL of acetic acid will produce 0.087 mole of isoamyl acetate (see the following section for details on how to perform this calculation):

$$5 \text{ mL x } \frac{1 \text{ L}}{1000 \text{ mL}} \text{ x } \frac{17.4 \text{ norm}}{1 \text{ L}} \text{ x } \frac{1 \text{ mole}}{1 \text{ norm}} = 0.087 \text{ mole}$$

The limiting reagent is the acetic acid: if there are only 0.087 moles of acetic acid, the maximum number of moles of isoamyl acetate that can be produced is 0.087 moles. Convert this mole amount to grams to get 11.3 grams:

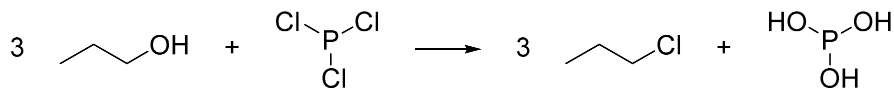
$$0.087 \text{ mole x } \frac{130 \text{ g}}{1 \text{ mole}} = 11.3 \text{ g}$$

To calculate percent yield, divide actual by theoretical yield:

$$\frac{3.21 \text{ g}}{11.3 \text{ g}} \text{ x } 100\% = 28.4\%$$

Example Problem 3

Three moles of 1-propanol reacts with one mole of phosphorus trichloride (PCl_3) to produce 1-chloropropane and phosphorous acid. What is the theoretical yield if you begin with 75 g of 1-propanol and 75 g of phosphorus trichloride? If you perform this reaction and isolate 96.3 g of 1-chloropropane, what is the percent yield?



1-Propanol | Phosphorous trichloride | 1-Chloropropane | Phosphorous acid

The stoichiometry of this reaction is:

- 1-propanol to 1-chloropropane, 3:3
- phosphorus trichloride to 1-chloropropane, 1:3

Since the stoichiometry of reactants to products is not 1:1, these ratios must be incorporated into the theoretical yield calculations (see below).

The physical data is:

Compound	**MW**	**Density**
1-Propanol	60.10	0.803
Phosphorus trichloride	137.33	
1-Chloropropane	78.54	0.891

75 g of 1-propanol will produce 1.25 mole of 1-chloropropane:

$$75 \text{ g 1-propanol} \times \frac{1 \text{ mole}}{60.1 \text{ g}} \times \frac{3 \text{ moles 1-chloropropane}}{3 \text{ moles 1-propanol}} = 1.25 \text{ moles 1-chloropropane}$$

75 g of phosphorus trichloride will produce 1.64 mole of 1-chloropropane:

$$75 \text{ g } PCl_3 \times \frac{1 \text{ mole}}{137.3 \text{ g}} \times \frac{3 \text{ moles 1-chloropropane}}{1 \text{ mole } PCl_3} = 1.64 \text{ moles 1-chloropropane}$$

Therefore, the limiting reagent is 1-propanol, and the theoretical yield is 98.1 g:

$$1.25 \text{ mole} \times \frac{78.5 \text{ g}}{1 \text{ mole}} = 98.1 \text{ g}$$

To calculate percent yield, divide actual by theoretical yield:

$$\frac{96.3 \text{ g}}{98.1 \text{ g}} \times 100\% = 98.1\%$$

6.3 Helpful Nomenclature and Relationships

The calculation of the number of moles of acetic acid (Example 2) brings up several questions that students often ask when encountering physical data involving acids. For acetic acid, you find in the table the MW, normality of concentrated reagent, the percent by weight, and the specific gravity.

1. Normality

Normality is the number of equivalents per liter, for an acid, an equivalent is the mass of acid that can furnish exactly 1 mole of H+ ions. The relationship between molarity and normality for several acids is summarized in Table 4.1.

Table 6-1: Molarity and normality.

Acid	Name	Relationship of molarity and normality
HCl	Hydrochloric acid	1 M = 1 N
H_2SO_4	Sulfuric acid	1 M = 2 N
H_3PO_4	Phosphoric acid	1 M = 3 N
CH_3CO_2H	Acetic acid	1 M = 1 N

2. Specific gravity

Specific gravity is the ratio of the density (in g/mL) of the compound at standard conditions relative to the density of water at the same conditions. Practically, you can assume that specific gravity equals density, therefore if concentrated acetic acid has a specific gravity of 1.05, it has a density of 1.05 g/mL.

3. Percent by weight

The percent by weight is the number of grams of the compound in a particular mass of the concentrated solution. If you have 100 g of concentrated acetic acid, you have 99.8 g of acetic acid. From this, you can calculate the number of moles using the molecular weight.

4. Which values should I use to calculate the number of moles of the acid in question?

The answer to this is: Whichever values you find more convenient, depending on which values you are given in the experimental procedure or measured in your experiment. If you are given a volume measurement, it is easiest to use the normality as in example 2 above. You could also use the specific gravity and the molecular weight to calculate moles from a volume measurement. If you are given a number of grams, you can calculate the moles from the % by weight and the molecular weight.

5. How do I calculate the number of grams when given the number of milliliters?

The answer is to convert using the following relationship of mass, volume, and density:

$$\text{mass} = \text{volume x density}$$

Density values are listed as grams per milliliter. For example, if you have 25 mL of a compound and its density is 0.97 g/mL, the number of grams is found by the following calculation:

$$\text{mass} = 25\ \text{mL} \times 0.97\ \text{g/mL} = 24.2\ \text{g}$$

6.4 Lab Report Format

The parts of a lab report are listed below. All of them must be typed, except the Data and Observations, which must be handwritten in a carbon-copy or carbonless lab notebook. All parts must be turned in as paper copies - email submissions will not be accepted. Make sure both the prelab and postlab are labeled with your name, lab section, and experiment title. **Example lab reports are available on the course website.** You may use these as a guide when writing your own lab reports.

A. Prelab – due at the start of that day's experiment

1. Introduction

In a sentence or two, state the purpose of the experiment. There are different types of experiments: technique and preparative. A technique experiment is one in which you are performing a technique for the first time and studying its details, for example, distillation and extraction. A preparative experiment is one in which your goal is to synthesize a compound from other reagents. For both these experiment types you should draw the chemical structures you will be working with. For a preparative experiment you should also show the mechanism by which the reaction will proceed.

2. Physical Data

In a table, list the name, MW, melting point, boiling point, density, solubility, and hazards (see Chapter 2) of all pertinent chemicals used in the experiment. Calculate the amounts of reactants (or compounds to be purified) in moles, grams, or mL as appropriate. In a preparative experiment, calculate the limiting reagent and the theoretical yield of the product. Be sure to include your calculations for these values. Refer to the Handbook for information on how to calculate yields.

3. Procedure

Briefly summarize the procedure to be followed, using numbered steps. You do not need to write out the procedure in complete sentences and you should not copy directly from the Lab Manual. All you need is a brief but complete listing of what you plan to do in the lab. The first time you do a technique, such as distillation, include in the procedure section a description of how to assemble the apparatus and how to conduct the distillation. In later experiments, it will be sufficient to state only that the liquid was distilled. In a research laboratory, you would need to cite the literature reference for the procedure that you are following; in the teaching labs, most of the procedures that you will follow are in the Lab Manual; therefore, a reference citation is not necessary. You will earn points based on completeness, correctness and how easy it is to follow.

B. Postlab – due at the start of following lab

1. Data and Observations

Your handwritten observations of the experiment as it progresses are important, new information. Write these observations (color changes, appearance of crystals, formation of an emulsion, boiling temperatures, test results, etc.) in your notebook as you do the experiment. Also record the weights of reagents and products and tare weights in this section. You do not need to rewrite the procedure; you should write things like, "Performed steps 1-4 as written. For step 5, weighed out 0.023 g of reagent A. At step 6, reaction was spilled and had to be started over." As a guideline, consider that from the procedure and observations sections, any chemist should be able to duplicate your experiment. With this in mind, be thorough but include only pertinent information. Be sure to label any data you write down – if the notebook is just a jumble of disorganized numbers it will be hard to interpret the data later.

2. Discussion of Results

This is the section in which you interpret the data obtained in the previous section. First, give a quick review of the procedure that you followed, including a brief explanation of why each step was performed – for example, why was it necessary to recrystallize your product? Did anything unusual occur or did everything go as expected? Then discuss the results of your experiment. For instance, indicate the amount of purified compound that you obtained and how the purity and identity of the compound was assessed. Calculate the percent yield (or percent recovery for a preparative lab). Include and discuss instrument printouts, such as NMR or IR spectra. In this section, you can state whether or not the procedure was a good method for making the desired compound; if not, try to make suggestions to improve the method for future experimenters. However, you should not use sentences like "This was a bad lab," "I enjoyed this lab," or "I think this lab worked well." Be specific and detailed in your feedback. This section must be written in 3rd person past passive tense. This means you should use phrasing like "0.023 g of Reagent A was added to the round-bottom flask, and the flask was heated to reflux," instead of "I added 0.023 g of Reagent A and then I heated the flask to reflux." Points are based on clear writing, correct yield calculations, correct spectral and data interpretation, analysis of error, and suggestions for improvement.

3. Technique

This is not a separate part of your lab report, but your TA will assign a technique grade based on your entire lab report as a whole. This is not necessarily determined by what yield you get or whether your reaction worked – it is based more on how prepared you were and whether you performed the lab correctly. Reading the assigned sections in the Handbook and following directions will dramatically increase your chances of getting a high technique score. If you try to perform the lab in a manner that makes it clear that you have no idea what you're doing, then you will probably lose some of the technique points. In addition, if you commit any serious breaches of the safety rules then you may lose all of the technique points, since you will be endangering yourself and others.

6.5 Drawing Chemical Structures

All chemical structures in your lab report should be drawn using a chemical structure drawing program such as ChemDraw. The chemistry department has a site license which will allow you to install a copy of this program on your computer for free. Instructions for downloading and installing ChemDraw are posted on the course website.

If you are taking 3321 or 3361 (nonmajors OChem 1 lab and majors OChem 1 lab), the first experiment will include an introduction to downloading, installing, and using ChemDraw. If you are taking 3341 or 3381 without having taken 3321 or 3361 at CU, you should contact the lab director for a copy of this experiment and work through it on your own.

Please do not hand-draw structures in your lab reports, and do not copy and paste images from websites either. You will lose points for doing either of these things. All figures in your lab reports should be your own work.

6.6 Plagiarism and How to Avoid It

Plagiarism means passing someone else's words or ideas off as your own, whether your source is the organic lab books, the internet, or other students. The purpose of having you write lab reports is to learn the skills needed to succeed in a technical or scientific field: clear descriptions, coherent writing, meaningful analysis of data, and understanding of the subject matter. Copying someone else's words will not allow you to build up these skills.

Plagiarism is forbidden by CU's Honor Code, and if you are found to be plagiarizing you will receive a grade of zero for that entire experiment and probably be reported to the Honor Code Office. It is your responsibility to avoid plagiarizing. This table will help you to recognize where the line is drawn between plagiarism and acceptable use.

Text	Source and verdict
A TLC plate is a sheet of glass, metal or plastic that is coated with a thin layer of solid adsorbent (usually silica or alumina). A small amount of the mixture to be analyzed is spotted at the bottom of this plate.	Original text (Chapter 12 of the Handbook)
A TLC plate is a sheet of material that is coated with a thin layer of solid silica or alumina. A small amount of the mixture that will be analyzed is spotted at the bottom of this plate.	This student has copied almost verbatim from the book. This is plagiarism.
To perform TLC, a small amount of the mixture to be analyzed is spotted at the bottom of a TLC plate. This plate is a sheet of glass, metal or plastic that is coated with a thin layer of solid adsorbent (usually silica or alumina). (Handbook for Organic Chemistry, pg. 124)	This student has also copied most of the wording from the book, although the order of sentences is switched. Even though the handbook is cited, this is also plagiarism.
TLC plates consist of a thin layer of adsorbent coated onto a solid support sheet. For the plates used in the undergraduate labs, the adsorbent is silica and the support is aluminum. To prepare a plate, a small amount of the analyte must be placed near the bottom of the plate using a TLC spotter.	This student has reworded the important ideas from the paragraph and added more specific information from the experiment. This is acceptable. A citation is not needed for information contained in the Handbook or Experiment Manual for this course.

To avoid obvious plagiarism, you should avoid copying and pasting. It's fine if you and a friend are sitting together working on your lab reports and discussing the key ideas, but you should not share any files with each other or copy text directly out of each other's reports. The best method is to read the source information and take notes that summarize the key points. Then, once you've decided which key points are relevant to your lab report, you can type up complete sentences that explain these ideas.