# Organic Chemistry Formal Written Laboratory Reports

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### Document Formatting

Document should be standard 8.5” x 11” with margins of 1”, 1”, 0.5”, 1” (left, right, top, bottom) and 0.5” header and 0.6” footer. Type face should be an easily readable font such as 12 pt Helvetica, Times, Times New Roman, or Palatino. Double space everything to allow for comments.

### Title

It is recommended that the title be written after the experiment. It should be brief and grammatically correct but accurate and complete enough to stand alone. The title should include keywords that might engage the reader. Avoid phrases such as “on the”, “a study of”, “report on” and “use of.” Don’t try to be tricky or fancy, just keep it simple.

### Abstract

This section is a complete summary of what was done and what was found. It includes an overview of the general methods and results. It does not include experimental details (e.g., “1 M $NaOH_{(aq)}$ was used”). It is written in the past tense and is a “stand alone” description of your work.

### Introduction

The purpose of this section is to stimulate interest and prepare the reader. It should describe the motivation and focus of experiment, why it is significant. It may contain theoretical background, chemical names, formulas, equations or structures. All information in this section should include references to the literature where the material was found. Wikipedia is not the best source of information, and should not be used as a primary source. This section contains a minimum of two paragraphs. The last paragraph is always a non-technical overview of the experiment.

The non-technical overview is an overview of what was done, in more detail than the abstract, but excluding things like temperatures, solvents, reaction times and the like. The non-technical overview does not include results.

### Methods and Materials

All reagents used should be listed and sources cited (Chemical 1, Chemical 2, Chemical 3 were obtained from the stockroom and used without modification). The make and model of instrumentation used for characterization should be reported here, including software for analysis. The procedure for the experiment is then given in condensed format. If the procedure was followed unmodified you may simply cite your lab manual, specifying sections that were performed (The procedure in Pavia et. al.[ref #] was followed without modification). Any deviations, additions or omissions to the reference procedure must be clearly stated here. The experiments designed by individual students must be described in a separate paragraph.

Your Mel-Temps are Mel-Temp II by Barnstead/Thermolyne model 1001 with a Fluke 51 K/J digital thermometer. The IR instrument is a Nicolet Avatar 360 FTIR ESP with Omnic 8 software by Thermo Fisher Scientific.

An example of what this section should look like is given below. We do not have all of this instrumentation, this is only for example.

> Bromobenzene, magnesium turnings, anhydrous diethyl ether, 6 M $HCl_{(aq)}$, and petroleum ether were obtained from the chemistry stockroom and used without modification. Melting points were determined using a Barnstead/Thermolyne Mel-Temp II model 1001 equipped with a Fluke 51 K/J digital thermometer. Infrared spectra were obtained on a Perkin-Elmer 1600 Series FTIR. $^{1}$H-NMR and $^{13}$C-NMR were obtained on a Bruker AC250 250 MHz NMR equipped with a quad nucleus probe, and in some cases on a Varian Unity500+ 500 MHz NMR. Chemical shifts are reported relative to tetramethylsilane in δ ppm. $^{11}$B-NMR spectra were obtained on a Bruker AC250 250 MHz NMR equipped with a quad nucleus probe. $^{11}$B-NMR chemical shifts are reported relative to $BF_3$-$OEt_2$ in δ ppm. Purity of the materials synthesized, unless noted otherwise, was assessed solely through $^{1}$H-NMR.
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> Fifteen milligrams of magnesium turnings (6.43 mmols) were placed into a 20-mL round bottom flask. The flask was fitted with a magnetic stir bar, a Claisen head with rubber septa, and drying tube. A solution of Bromobenzene (1.01 g, 6.43 mmols) in anhydrous diethyl ether (4.0 mL) was added to the stirred reaction flask via syringe dropwise. Addition of bromobenzene/diethyl ether solution was maintained at a rate to produce a steady reflux of the reaction mixture. After addition of bromobenzene/diethyl ether solution, the reaction was allowed to cool to room temp. A solution of benzophenone (1.09 g, 5.98 mmols) in anhydrous diethyl ether (2 mL) was added rapidly via syringe. The reaction was allowed to stir for 20 min. The reaction mixture was quenched with $HCl_{(aq)}$ (6.0 mL). The resulting biphasic system was separated using a separatory funnel, and the aqueous phase extracted with 10 ml diethyl ether. The ether layers were combined and evaporated to yield a yellow solid/oil mix. The solid was triturated with petroleum ether and filtered to yield the crude triphenylmethanol (1.25 g, 4.80 mmols) as a white powder. The crude material was recrystalized from isopropanol to afford the pure triphenyl-

methanol. Yield: 1.04 g, 4.00 mmols (67%). Mp. 160.5 – 161.0 $^{o}$C. FT-IR (Solid, KBr pellet, $cm^{-1}$): xxxxx, xxxxx, xxxxx, xxxxx (where xxxxx are the important wavelengths for characterization).

**Results**

This section includes data tables, graphs and sample calculations. All tables and graphs will have appropriate titles and be a half page in size. The axes of the graphs will be properly labeled including units. Results should be summarized in text as well as tables. I know it's redundant, but that's only because our data sets are rather small.

**Discussion/Conclusion - These may be treated as one or two separate sections**

For organic papers, the first part of the discussion should be about the reaction mechanism. This is not a hard rule. If the mechanism is very small it can be placed in the introduction section. Likewise if there are topics to discuss that could come before the mechanism it is fine to do so.

The mechanism should be broken down into individual reaction steps. Each step should be proceeded by a figure and caption illustrating the step. The text should then explain what is taking place. The figures can be hand drawn, as can the caption headings. Computer drawn images are really nice but take a long time to master. There are a number of free applications for Macs and PC's that will allow you to draw molecules, however I would rather have you focus on other areas of the report and simply draw the reaction diagrams by hand. Just leave space for the figures in the text and add them afterwards.

In addition to the mechanism the discussion section is generally where the results section is thoroughly integrated to produce sound conclusions. Critical thinking is employed to analyze the results and deduce valid conclusions. In organic chemistry this section should include a discussion of any experimental difficulties, errors, or questions. It may also include answers to lab manual questions. In fact I would recommend looking at the lab manual questions and using them as an outline with which to construct this part of the discussion.

The Conclusion section is very brief, usually a single paragraph. Most often I think of this as a restatement of the abstract. Don't just copy the abstract however. The conclusion should reaffirm what was done and what was found. Sometimes, comments regarding future experiments may be appropriate.

**Language and Format**

In general, the report is written in the third person, impersonal observer voice. For example, "Ten grams of NaOH was weighed", **not** "I weighed 10 g of NaOH."

Using “we” or “I” in a lab report is very rare, it only pertains to comparison with others’ results.

Reports should be typed. Equations, calculations and structures can be written by hand even in a type written report. If chemical formulas and equations are not handwritten they must be formatted correctly using the appropriate sub- and superscripts.

**Figures, Charts, Schemes and Tables**

Graphical images fall into several types: figures, charts, schemes, and tables. Each graphical element should be referred to properly and most often addressed with a caption.

Captions are titled as “Figure 1.”, “Chart 5.”, “Scheme 7.”, or “Table 2.” followed by a period and then a description of the item. The caption is generally 2 pt smaller than the body text and indented both left and right of the body paragraph. Each caption is numbered sequentially within that graphical image type. For instance, you may have figures 1 through 8 and then wish to place two tables, which would be table 1 and table 2. The next figure would be figure 9.

A single structure or formula does not need a caption. This is often used when a single molecule is desired to be shown.

Figures are single structures, apparatus illustrations or graphs of reaction data for which the caption is placed below. Single mechanistic steps can be either figures or schemes, however most journals generally refer to them as figures.

Charts are collections of structures for which the caption is placed below.

Schemes show action such as full reaction mechanism or flow chart for which the caption is placed below.

Tables are collections of data or results for which the caption is placed at the top of the table.

**References**

References can be done either as footnotes or endnotes. References are cited within the text differently depending on the specific Journal. We will use a superscripted number directly following the information cited. This can be mid-sentence[1] or at the end of the sentence.[2] The references should be sequential in order of use, however a reference can be used more than once. For instance, after using a reference in the introduction as reference 3, it is okay to invoke reference 3 again in the discussion even though the next unique reference may be 9. Reference formats depend on the type of information referenced as illustrated below.

Books[1] - Author Last Name, Middle Initial. First Initial.; Second Author Last Name, Middle Initial. First Initial. Chapter Title. *Book Title;* Publisher: Publisher location City, Country, **Year**; pages.

Journals[2a-c] - Author Last Name, Middle Initial. First Initial.; Second Author Last Name, Middle Initial. First Initial. Article Title. *Journal Title*. **Year**, *Volume*, Pages.

Patents[3] - Author Last Name, Middle Initial. First Initial.; Second Author Last Name, Middle Initial. First Initial. Patent Title. Country and Patent Number, **Year**.

Web Pages[4] - Title of Web Page. http://address (date accessed - Month, **Year**), Navigational Submenus utilized.

**Additional Information**

Additional information on general formatting, references, correct usage of chemical symbols, contents of scientific papers, scientific writing tips and more can be found in the ACS Style Guide, Second Edition[5], and in A Short Guide to Writing About Chemistry by Davis, Tyson, and Pechenik.[6]

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1. Collins, P.; Ferrier, R. Preliminary Matters – Structures, Shapes and Sources. *Monosaccharides: Their Chemistry and Their Roles in Natural Products*; John Wiley & Sons: Chichester, U.K., **1995**; pp. 40-44.

2. a) James, T. D.; Sandanayake, S.; Shinkai, S. Saccharide Sensing with molecular receptors based on boronic acid. *Angew. Chem. Int. Ed. Engl.* **1996**, *35*, 1911-1922. b) James, T. D.; Linnane, P.; Shinkai, S. Fluorescent saccharide receptors: a sweet solution to the design, assembly and evaluation of boronic acid derived PET sensors. *Chem. Commun.* **1996**, 281-288. c) James, T. D.; Shinkai, S. Artificial receptors as chemosensors for carbohydrates. *Top. Curr. Chem.* **2002**, *218*, 159-200. d) Hartley, J. H.; James, T. D.; Ward, C. J. Synthetic receptors. *J. Chem. Soc., Perkin Trans. I* **2000**, 3155-3184.

3. Sundrehagen, E. (Axis Research AS, Oslo, Norway) Glycosylated haemoglobin assay. U.S. Patent 5,242,842, **1993**.

4. American Diabetes Association Home Page. http://www.diabetes.org (Aug **2002**), Basic Diabetes Information, Facts & Figures, Impact of Diabetes.

5. Dodd, S. J.- editor. *The ACS Style Guide: A Manual For Authors and Editors, Second Edition*; American Chemical Society: U.S., **1997**.

6. Davis, H. B.; Tyson, J. F.; Pechenik, J. A. *A Short Guide To Writing About Chemistry;* Pearson: New York, U.S., **2010**.