Lab Report Help Sheet – Chemistry 381

Lab reports should have the following sections: Abstract, Introduction, Results & Discussion (two sections that are often combined into one), Experimental, and References. In addition you will want to put in a title. This division of sections follows the standards set forth by the American Chemical Society. Other journals (non-American chemistry or other scientific fields) may format their articles differently. I tend to think of journal articles as being as short as possible. You should take the time to say everything necessary but do not put in a lot of fluff.

To make things as simple as possible, we will use a *template file* from the *Journal of Organic Chemistry*. (Our template file is not *exactly* like the one for *J. Org. Chem.*, but it is pretty close.) Template files make things easy – just type the text into the correct area and the template will make sure it is properly formatted. Of course, one needs to know what text goes where.

One important part of a paper is its figures and schemes. A figure shows molecules – not reactions, just molecules. For example, a figure might show different drugs that treat a certain condition. Schemes show transformations of molecules, including reactions or mechanisms. (Figures and schemes *always* follow their mention in the text. Place figures after a paragraph, not in the middle of it.) For our report, we will use a program called ISIS/Draw (available as a free download if you register at http://www.mdli.com/download/idrawdown.html). When making figures with ISIS/Draw, you must apply the appropriate settings from the Options menu (Read Journal or Custom Settings… JOC.CFG). Figures and schemes created in ISIS/Draw can be copied and pasted directly into Word documents.

Three sample papers show off how to write a paper. Look over these papers. Examine their language. Look at the various parts of the papers and compare each part to the section descriptions listed below. Become acquainted with how researchers put together a paper.

http://pubs.acs.org/cgi-bin/article.cgi/joceah/2008/73/i20/pdf/jo8002562.pdf
http://pubs.acs.org/cgi-bin/article.cgi/joceah/2008/73/i20/pdf/jo8015743.pdf (Snyder paper)
http://pubs.acs.org/cgi-bin/article.cgi/joceah/2008/73/i19/pdf/jo801269m.pdf

Abstract
This is a very short synopsis of your experiment. Most abstracts are little more than a handful of sentences giving a minimal description of the experiment performed with final observations. The abstract will probably not mention any topics discussed in the introduction. More is not better with an abstract. Basically, you need to say what you did (like make a target molecule) with the final result (such as percent yield). In our sample papers, the abstract appears between two horizontal lines at the start of the paper. Do **not** create a graphic for your abstract, and do **not** refer to compound numbers from other figures within your abstract. The abstract will be pulled by abstracting services, like Chemical Abstracts. Chem. Abstracts will not include any figures in the abstract, so do not confuse the reader by putting in compound numbers. The abstract is a stand-alone part of the paper.

Introduction

Also frequently called the background section, the introduction is normally fairly short. The introduction presents general interest information on the chemistry, and should on some level justify the entire experiment. The introduction should answer the questions, "Why did you do these reactions and why are they important?" If we had made a dye in lab, an appropriate introduction might be to discuss the importance of dyes in daily living. (Dyes are important, and to demonstrate their synthesis, we made a dye. – a one sentence introduction!) Our first lab report is on the aldol condensation. You should give a short paragraph (three or four sentences) on the aldol condensation, its uses and importance. Normally, an introduction section contains a figure or scheme that accompanies the text. Do not lose sight of the fact that the paper is about your experiment, not the introduction. The introduction merely sets the table for the presentation of your results. An introduction almost always concludes with a single sentence that describes the work performed in the results section. This sentence bridges the background (introduction) and the work performed (results). This sentence often stands out because it is the one line in the introduction that uses first person voice.

Results and Discussion

The results section tackles what you did for each experimental step with any significant observations. One or two sentences per step is sufficient. You should not go into great detail; data such as R_f or melting point does not belong here. You should definitely give a complete reaction scheme. In your scheme, number the compounds in the scheme and use these numbers when referring to the scheme (*i.e.* if the final product is an aniline and numbered **6** in your scheme, you might refer to it as aniline **6** or amine **6** or even compound **6**). Just give a quick description of what you did and leave the rest for the discussion. For a synthetic paper like yours, the results section will likely be only a paragraph – maybe just a very short paragraph. If an experiment completely failed, then that would be the result – a 0% yield of the product was obtained.

A comment on compound numbers – Be careful with compound numbers. There are two ways to use them: with parentheses and without parentheses. Use numbers with parentheses when the number is needed for the sentence to make sense. For example, we made amine **1**. Without the number, the sentence does not work. Use parentheses when the number is not needed for the sentence. For example, we made benzylamine (**1**). In this case, the number serves as a reminder to the reader and says, "We made benzylamine, and, by the way, benzylamine has the structure of compound **1**."

In the discussion section, you *discuss* what happened. For a total synthesis project like ours, the discussion could be very short. The goal was to make a compound, and you made that compound. However, if any problems were encountered, they will need to be addressed. What went wrong? How do you know something went wrong? Do you have any ideas on what caused the problem? Do not turn this into a huge essay, but you will need to answer these questions. Similarly, you should address what went right. Was the reaction a success? How do you know? – Was the product pure? (by what measure). Note that this is mostly your *interpretation* of what happened. The results section is more factual. The discussion becomes more opinion.

Conclusion
There is not a lot to say here. Basically, do a *very* brief recap of the discussion. Once again, you wanted to make something, and you made it. For hard-core research papers, the conclusion is much more important than for us.

Experimental
Your experimental will be divided up with a small section for each compound you made. We only made one compound, so we'll just have one section. For each, provide the full IUPAC name. Following the basic format used the example papers, give your experimental procedure. Each procedure should be brief. At the end of the procedure list any physical characteristics (R_f of TLC and mp). For NMR data list the chemical shift, peak multiplicity (singlet, doublet, etc…), relative integration (1H, 2H, etc…), and the coupling constants (*J*-value). At a minimum an experimental should list a brief procedure noting things like amounts used, temperature, time, etc…, the characterization data (MP, TLC, NMR), and the yield of that particular step.

Of our sample papers, the one by Snyder at Brandeis has the most helpful experimental section for us. Note that Snyder's experimental procedures are very concise. You should be concise too. Do not be as verbose as the lab handout. Also, follow Synder's example of how to report your experimental data.

References
Throughout your report you will likely occasionally need to insert a reference. Number each reference and collectively list them (numbered and in order) in this section. Unlike a professionally typeset journal article, we won't use footnotes. References you will likely need include any sources for melting points, the source of the experimental procedure, and anything else you used in putting your report together. You may need references for your introduction. Note that the references are inserted into the text as superscripts at the end of phrases or sentences. The superscripts should be placed *after* punctuation, not before. For example, this is incorrect[1], while this is correct.[1] The first superscript should follow the comma. As always, look at the formatting in the sample papers, which follow the ACS style.

Hints to a Decent Lab Report

- A lab report is not a way for chemistry courses to make you write a paper. A lab report should *objectively* and *concisely* present a series of experiments. It will not be a masterpiece of English prose. On the other hand a report should be well written.
- Look at the sample papers. They are mostly in third person passive voice. It is OK to use first person active voice, but do not go crazy with it.
- Write your abstract first. When you get stuck, use your abstract to guide you on what you need to say next. When you are done, your report and abstract should fit together.
- If you question whether something can be left out or not, it can probably be left out. Do not take this as an excuse to hand in a one-page report. Only include topics that need to be addressed from a scientific standpoint. The exception to this rule is the introduction. Extra details like this are interesting when in the introduction, but they are out of place in any other section.

- Be warned that it will take a bit of time to get the hang of ISIS/Draw. A poorly drawn computer structure is just as ugly as poorly drawn freehand structure.
- When you are completely lost, consult the example papers. These were specifically chosen to give you an idea of what to do. Use them! Look at how they do things like incorporate the introduction or briefly go through the reactions in the results section. Follow their lead.
- A comment on compound numbering: Each structure in your figures and schemes should be numbered so that you can reference it by number in the text. Assume you number an alcohol as compound **2**. You could refer to that compound as alcohol **2** or compound **2**. Sometimes people put numbers in parentheses. If the number is in parentheses, you should be able to remove the number and still have the statement make sense. An alcohol (**2**) was the desired product. In contrast… Alcohol **2** was the desired product. When the number is not in parentheses, it is required for the sentence to make sense. Please refer to the sample papers!