Notebooks and Reports
Writing in the Physical Chemistry Laboratory Courses

"Without publication, science is dead."
- Gerald Piel

To be an effective scientist, you must be able to tell other people what you are doing, in a way that will make them want to listen. Often this takes the form of writing, be it scientific articles, grant applications, reports to committees, etceteras. Your writing will almost always be subject to review by other scientists and/or other professionals. In the scientific community, this is called peer review, and forms the basis for the publication of articles, funding awards, promotion, and many other achievements. Since you will also be a peer, you are likely to review almost as many pieces of other scientists' writing as they review for you!

In this course, you will develop your skills in scientific writing and critiquing (both of your own work and others') by producing both laboratory reports and a scientific article. While they share many similarities, a laboratory report (see **section C**) differs somewhat from a scientific paper written for publication in the audience and principle goal of the writing. A laboratory report is intended to demonstrate your understanding of the material and the mechanics of its analysis to your professor, while a scientific paper (see **section B**) is intended to communicate something new and to describe its relevance to what is already known to your peers. You will gain experience with both types of writing in this course. Near the end of the semester, you will also perform a peer review on a classmate's scientific article, and receive several peer reviews from them on your article (see the *Sample Peer Review Form* for an idea of how an article is reviewed). As in the "real world", these comments should be helpful to you in revising your article for final submission.

At the heart of all good research is a good lab notebook (see **section A**). The integrity of a piece of work lies in the details, and hopefully the details lie in your lab notebook. Therefore, you should also expect to spend considerable effort on keeping a good lab notebook. In fact, the bulk of your laboratory reports will consist of your notebook records.

Before beginning to write your first report, read the section on report writing in SGN[1] (p.10-24). You may also find it useful to periodically refer to *The ACS Style Guide*[2] (Ch. 1-3 in particular), and Moore's *Writing to Learn Science*[3], which are on reserve in the library. When you are ready to draft your final article, you will need to consult the *Instructions for Authors* section of this manual for detailed formatting guidelines.

Even for the best of writers, effective writing requires writing and rewriting, thinking and rethinking, learning and relearning - i.e.: it requires **time** and **energy**. *Do not* leave the writing of a report or worse, your article, until the last minute!

A. The Lab Notebook

A good lab notebook contains **everything necessary for the duplication of your experimental results by an outside chemist**. In this course you will be keeping a notebook

[1] Shoemaker, D.P., Garland, C.W. and Nibler, J.W., *Experiments in Physical Chemistry* 6th Ed., McGraw-Hill (1996)

[2] Dodd, N. S., Ed. *The ACS Style Guide*, ACS, Washington DC (1986)

[3] Moore, R. *Writing to Learn Science*, Saunders Publishing, Forth Worth (1997)

geared towards chemists at your level. What you do, observe, measure, calculate, and conclude[4]. must be recorded accurately and descriptively so that another classmate who is not taking the class could understand what you did and reproduce the results from your notebook alone. This does not mean that you have to write a novel every class period! It does mean that you need to be organized and write down what you do as you go. Some guidelines are listed below. There are also several examples of good laboratory notebooks available on reserve in the CHEM313 binder in the Lab Room (CH455). Be sure to follow the same guidelines when you work on your independent project.

Your lab notebook is your intellectual property and its contents stand up for you – right now it will give you credit for this course. Later, a lab notebook may give you a graduate degree, scientific recognition or perhaps a patent. At the very least, a good lab notebook testifies to the effort you have put forth. A poor lab notebook has been known to get people into very hot water.

The Notebook Itself:

We will use the same guidelines for keeping a notebook that are used in graduate research labs and industry:

- Your lab notebook must be hardbound with numbered pages. Spiral notebooks or those with perforated tear-out pages are not acceptable. On the inside cover, write your name, course number, and phone number in case the notebook gets lost.
- Leave the first few pages blank for a table of contents. Otherwise, leave no blank pages in the body of the notebook.
- Write the date at the beginning of every new entry. All entries must be made in indelible, waterproof pen. Any mistakes should be drawn through with a single line.
- For this course, please write directly on the pages that tear easily, on every other line (**double-spaced** - this leaves room for comments). This may mean that your carbon and original copies have different page numbers. Penmanship *is* important! If no one can read your notebook, then the experiment is not repeatable.

Before Each Experiment or Lab Day:

To complete experiments on time, you must be prepared before you come to lab. This means that you should know what you will be doing and why you will be doing it. This will allow you to make a rough check on your data as you collect it and make adjustments if necessary. Therefore, you must **do the following things before you come to lab**:

- Enter the date and a title for the experiment on a new page. Choose a title that describes the essence of the experiment as you understand it (this is *not necessarily* the title from the lab handout or textbook). Your title may change later – that's ok.
- Write a short overview of the experiment in your notebook. This should include the purpose of the experiment, a brief description of the theoretical background needed to understand the essence of the experiment, a brief description of the experimental plan, and a

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[4] In an industrial research notebook, conclusions are not usually recorded so that patent applications are not limited by your particular interpretations.

brief description of the calculation route. This should be no more than about three pages (double-spaced).

- Complete any derivations that are indicated in the experiment description by the "⇨" symbol.

During the Lab:

(See also the section in SGN (p. 7-9) on recording experimental data.) As you perform the experiment, enter in your notebook:

- your experimental setup (a sketch is better than a long paragraph if the setup is complex)
- the **details** of the procedure
- your observations, and
- any measured values, with **units**.
- write out clearly all calculations that you perform (even dilution calculations), **with units**.

You do not need to include details such as "I walked across the lab to get the solvent", or "The volume was read by looking at the bottom of the meniscus" – assume that your peers have the same experience that you have coming into the course. However, writing units with values as you work calculations is an *extremely important* habit to get into. As an example, several years ago, NASA lost the Mars Explorer because the engineer that performed some last minute calculations did so in one system of units (SI or British), but the rest of the engineers assumed that he had done so in the other system of units. The trajectory of the Explorer as it aimed towards Mars was therefore wrong, and resulted in the Explorer bouncing off into Outer Space. This was clearly a very expensive mistake …. don't let it happen to you! I strongly suggest that you perform a crude "back-of-the-envelope" (but in your notebook) work up of your data as you acquire it so that you can assess your technique and make adjustments if necessary.

Most importantly, keep in mind that ***your notebook is not scratch paper!*** You need to

- include enough **narrative** so that the context of the measurements and calculations is clear
- organize your data so that it is easy to read

This does *not* mean that you need to write a short story – an outline (bullet or list) form is often easiest to read. Numerical results (both raw and final) should be recorded in an organized manner (in a table, for example), include units, and be written with the appropriate number of significant figures. You should also include an estimation of the error if possible.

When you are finished for the day, have your instructor sign your notebook.

Data Workup:

In order for someone else to understand what calculation you are performing, they must be able to see the equation that you are using. Therefore, before you begin to crank through the math,

- indicate the context of the calculation (what are you calculating?)
- write out the equation and define all variables
- rearrange it to solve for the variable of interest.

Only then may you substitute values, **including units with every number** (this is not optional, see above). Check the units on your final answer using dimensional analysis to be sure that you have rearranged the equation correctly. Report final values to the correct number of significant figures as indicated by your error analysis. Clearly highlight (with boxes or otherwise) results that you feel are important.

Calculations that are performed on a computer are not exempt from notebook-keeping (computer-aided workup can actually involve *more* record-keeping!) Simply printing a copy of the spreadsheet or graph is not sufficient. You need to explain your logic in processing the data and include enough information so that another person who is familiar with the software could reproduce your results. Some details to keep in mind as you perform the workup on computer are given below:

- Explain your logic in attacking the problem. This includes the nature of the calculations, the details of plotting, and any other data processing details that will not show up on printing or are not the default settings (for example, forcing an intercept to be zero). Be sure to include units in your documentation! **Record the final results of calculations or graphical analyses (including units) in your notebook.**
- Print out and include any useful tables or graphs with your notebook record (you may want to print two copies: one to hand in and one for yourself). If you are working with Microsoft Excel, you must print two versions of your spreadsheet: one with the values shown, and one with the formulas shown (exceptions will be announced in class). **All spreadsheet printouts should include row and column headings.** To print these, select Page Setup, click on the Sheet tab, and select Print row and column headings. To print the hidden formulas, select the "View…Formulas" Option under the Tools menu before printing. If you are working with Igor Pro, print out copies of both the Command and Procedure windows. However, please conserve paper in all cases and reduce the print size.
- **Always save a copy of your work to BOTH the hard drive and a floppy diskette!** On the hard drive, save all of your files in a folder with *your name* within the "Student Files" folder. If you decide to use password-protection on your files, you must **register your passwords with me**. It is a good idea to also record the filename and password in your notebook.

B. The Scientific Article (Independent Research Project)

The most interesting pieces of writing are those that tell a **clear** story in an **organized** way, and that have a **narrative** that is pleasant to follow. Your first order of business when you write a any paper is to decide on the story line. Scientific papers do *not* have to follow a chronological story line (in fact, this is often the worst story line to follow). Instead think about the following questions:

- Why are you doing this experiment?
- In what way is the laboratory procedure connected to your final goal?
- How is your final result connected to the body of physical chemistry knowledge?
- What kind of background information is needed to understand and appreciate your results?
- Who is your audience? How can you interest them in this story?

For this course, you may treat your audience as a chemist at your level who has not taken this course.

When you do start to write, do not worry about style, brevity, elegance, and etceteras. Just get your ideas down on paper (or screen). Then go back and **revise**. Ultimately, your final product should be both thorough and concise: each word should be significant. We are not used to using words this carefully in our everyday lives, so you must allow yourself time to think and revise. **Revise more than once**. Most scientists will revise a paper at least **10 times** before submission to a journal or grant agency for peer review!! Above all, you must hand in a professional-quality document: be sure to **proofread** your report for spelling and grammar mistakes! Papers that are submitted with egregious spelling, typographical or grammar errors will be returned unread and un-graded.

Formatting instructions for submission of papers to the *Journal of Physical Chemistry Lab* can be found in the *Instructions for Authors* section of this laboratory manual.

Sections of a Typical Scientific Article:

The traditional scientific paper contains 8 sections (although this varies from field to field and journal to journal): title, abstract, introduction, experimental procedure, results, discussion/conclusion, references, appendices. Organizing your data, ideas, and results so that everything is in the right place and tells the best story is usually a challenging task that takes revising and re-revising. Please plan ahead and start early!!

A. **TITLE:** The title presents the main point of the paper, and must be able to stand alone (i.e.: tell the essence of the story without the body of the paper). A good way to come up with a title is to make a list of key words (words that represent the main subjects of interest), then combine the most important key words into a statement about the experiment. Sketch a title out before you begin your report, but be sure that the title still represents the main point of the paper when you are done. A few other points of advice in choosing a title are:

- Make the title **specific** and **informative**, do *not* simply choose the name of the experiment (someone is not likely to gain much insight from a title like "Electronics Lab").
- Do not use abbreviations, jargon, proprietary names or chemical formulas. Do not include literature references or references to your paper.
- Be **complete** but **concise** – titles much longer than a line and a half are probably too long.

B. **ABSTRACT:** The abstract is a very dense summary of the paper, which must also be able to stand alone from the body of the paper. It is traditionally quite short (no more than ~300 words), and is best written last. As a general rule, equations are not given in an abstract, and references are to be avoided if possible (if necessary, the full citation is given in parentheses). All abstracts should include the following pieces of information:

- **context** of the study (generally no more than one sentence)
- **what** was measured/calculated (purpose)
- **how** it was measured/calculated (method)
- **key results** and **error** estimates, reported to the correct number of **SF**, with **units**.
- main **conclusions** and **insight gained.**

C. **INTRODUCTION:** The introduction serves to outline the **purpose** and **relevance** of the investigation. This means that you will have to survey some of the literature and find out what people know already. If you end up working on an already solved problem, your goal in the introduction will be to outline why this problem is interesting: what does it help you to learn, what is the extension from the experiments that you have already performed, and what have people already found out? Maybe they are wrong, and you will do a more careful study! In any case, a well-written introduction section will proceed from the general to the more specific, and should include ~5-10 references to previously published work. Usually introduction sections are no more than 3-4 paragraphs long.

D. **EXPERIMENTAL PROCEDURE (METHODS):** This section is a summary of **how** you measured your data and the theory that you used to process the results. The actual presentation of results is left to the Results section, and the interpretation of the results is placed in the Discussion section. Try not to blur these distinctions. Keep in mind that this is only a *summary* of your notebook record – it should include only enough detail for an experienced scientist to reproduce the results. I suggest that you read over several journal articles to get a flavor for a typical experimental section. Plan to include at least the following:

- make and model of any instruments used,
- important conditions such as temperature or sample concentrations,
- essentials of the procedure, including any special handling conditions (i.e.:, "cell was filled to the top and covered with parafilm to prevent degassing of bromine", or "the bomb was purged with 30 atm of O_2 to remove any residual nitrogen from the air", etc.),
- essential equations (see below) and an explanation of their relevance to your data workup. You do not need to derive every equation, but the connection between the ones presented should be made clear.

One component of a professional quality paper is appearance – this includes the use of conventionally formatted equations. Microsoft Word is available on all computers on campus, and is equipped with an equation editor (use Insert... Object… Equation). All equations must be formatted using this equation editor, must be numbered sequentially, and must appear on a separate line from the bulk of the text. All variables in equations must be defined within the text.

Common mistakes to **avoid** are:

- Giving instructions or writing lists of directions. Write what you ***did***, in the past tense and with the third person
- Using slang or jargon.
  BAD: The sample was measured using a spec at λ=254 nm.
  GOOD: Visible absorption spectra were obtained using a Spectronic 21 UV/Visible spectrometer at a wavelength of 254 nm..
- Writing the experimental procedure in excessive detail.
  BAD: The sample cup was weighed on an analytical balance, then a sample of benzoic acid was removed from the jar and placed in the cup. The cup was re-weighed and the entire cup/sample assembly was placed inside the bomb compartment. The electrodes were attached and the lid was screwed on. *Etc.*

GOOD: Samples were pre-weighed before assembling the bomb apparatus. (Although even this detail is probably not necessary to include.)

E. **RESULTS:** The Results section is the heart of any scientific paper. The early sections of the paper describe how you got to the results, and the later sections describe what the results mean. Without a good Results section, the rest of the paper is weak.

The Results section is comprised of a **verbal description of your investigation** along with **a summary of representative data in Tables and Figures**. Use narrative to lead the reader through your data work up – remember that you are telling a story. Several keys to writing a good Results section are indicated below.

- Present the results in an orderly sequence that corresponds to the order presented in the Experimental Procedure section, and the progression of raw data to final results.
- Construct your Tables and Figures first (see below) and use these as a basis for writing the Results section. Refer to Tables and Figures by number (they should be numbered sequentially as they appear in the text) and point out what is interesting and relevant in each Figure and Table.
- Present only representative data in Tables, Figures, and text. If there are multiple sets of data that are worked up the same way, present one or two examples, then summarize the results in a Table.
- Use a good topic sentence for each paragraph. The reader should be able to get the gist of the Results section by reading only the first sentence of each paragraph.
- Use statistical tests and/or error analysis to support general statements.

Common mistakes to **avoid** are:

- listing Tables, Figures or equations with no narrative or connection to the experimental section
- presenting overly raw data (i.e.: Temperature versus time data for a bomb calorimetry run)
- discussing the *interpretation* of the results in this section
- describing or repeating the *experimental methods or procedure* in this section
- using a whole sentence to refer to a Table or Figure. (Instead, state what you want to illustrate, then refer to the Table or Figure in parentheses.)
- using Table and/or Figure titles that simply recite the axis labels or type of data plotted

F. **FIGURES AND TABLES:** Read Chapter 3 of *The ACS Style Guide* and the section on *Instructions for Authors* for detailed format and content guidelines for Tables and Figures. Some essential components are listed below.

Figures:

- A **Figure Legend** is placed *below* the figure, and describes the information contained in the figure (one to two sentences at most). Do not simply repeat the axes labels! The reader should understand why you have included this figure in the paper from the legend alone.

- The **Axes** should be chosen so that **y** is the dependent variable and **x** is the independent variable. Chose axes limits that best feature the result - zero is not always important!
- The axis **Labels** must include units.
- Include a **Symbol Legend** *only* if there is more than one type of symbol or line on the plot. Choose symbols and line types that are easy to read in back and white print.
- Do **not** use a colored background for the plot area.

Tables:

- A **Table Title** is placed *above* the table, and describes the information contained in the table (one short sentence at most). Do not simply repeat the table column or row headings! The reader should understand why you have included this table in the paper from the title alone.
- The **Columns and Rows** of the table should be chosen so that similar elements are placed in columns. The leftmost column is the reference column to which all other columns refer (the row headings).
- The column and row **Headings** should be brief, descriptive, and include the units of measurements. The row headings are contained in the leftmost column.
- Present all numerical data with the correct number of **Significant Figures** and with **error limits**. Use leading zeros for numbers less than one (i.e.: 0.85 m, not .85 m).
- Use **Footnotes** to explain details that cannot fit in the headings (i.e.: literature sources, explanation of abbreviations, experimental details that apply to only specific entries, etc.).

G. **DISCUSSION/CONCLUSION:** The discussion is where you must **interpret** your results in light of the theoretical background and the work of others (which in our case will be "literature data"). This is where you communicate to the scientific community the "**insight**" part of the experiment. Here are some questions to keep in mind as you write the discussion:

- What is the physical meaning of your results? Do they support the your hypotheses? How do they relate to your introduction? What are the generalizations, relationships, and/or principles that are illustrated by your results? Connect your results to the theory.
- How do your results compare to what is already known? Are there similar situations to the one that you have studied that produce the same or different results (for example, the kinetics of a similar reaction, or the resonance energy of a similar molecule, etc.)?
- Explain the underlying causes of any significant discrepancies between your results and the literature or expected values. What assumptions have you made? Are they valid, based on your results?
- Are there flaws in the experimental design? Is the equipment is limiting the quality of your results? If so, what would define a better instrument? Discuss your error analysis - what parts of the experiment lead to the greatest error? Do you have grounds for suspecting any systematic error? How would systematic error influence your final results (a numerical estimation is best)?

All stories need an ending! Be sure to "wrap up" your discussion.

H. **REFERENCES:** At this stage in your career it is unlikely that you designed the experiment on your own, referred to no textbooks, and used no literature data. In fact, there is no scientific communication (be it written or oral) that does not include references! This is because it is unethical to use someone else's intellectual property without acknowledging their contribution, and it is a waste of time to be constantly re-inventing the wheel and not take advantage of past work. The bulk of your citations will probably occur in the introduction and discussion sections, although if you used the literature to come up with an experimental procedure, you should be sure to use citations there also.

Each source appears in two places in a paper: once in the body of the paper (the citation) and once at the end (the reference). Within the text, the source should be indicated – we will use a number in parenthesis *(1)* at the citation. In the References (or sometimes Bibliography) section, the source number is given, followed by the full reference. See the section on *Instructions to Authors* for examples.

I. **APPENDICES:** Because this is a course, your notebook pages will be submitted with your article, but do not consider them an appendix. Rarely do scientific articles contain appendices at all. If they do, it is usually tables of raw data that have been requested by a reviewer or a lengthy derivation. You should not need to include an appendix with your paper. If you have questions about it, please see me.

C. Laboratory Reports (Laboratory Experiments from this Manual)

The traditional report is modeled after a scientific paper and contains the same 8 sections. However, since you will be spending a significant amount of time drafting a scientific article later in the course, the laboratory reports for CHM313 will be truncated versions of a scientific paper, which contain only the following sections in addition to your notebook pages: **title; abstract, references, appendices.** The reports are designed to get you thinking about the science and to give you some writing practice before your article is due. Therefore, they should be taken seriously and be something that you take pride in when submitted.

Sections of a CHM313 Lab Report:

A. **TITLE PAGE:** This typed page (**double spaced**) must contain:

- The **Title** of the report (see guidelines above)
- **Your Name**
- your **Lab Partner's Name**
- An **Abstract** (see guidelines above).

B. **NOTEBOOK PAGES:** Your notebook record will make up the body of your report. It therefore will save you a lot of time if you get in the habit of writing in your notebook as you go, in an organized and complete way. The sections of your notebook for each experiment should be:

- The **overview** that you wrote before you began the experiment (like an Introduction)

- **Experimental details**, including the procedure and any calculations performed during lab periods (like an Experimental section).
- **Data workup**, including calculations, tables, plots, final results, etc. (like a Results section).
- A short **discussion** of the results, no more than ~ 1 page (like a Discussion section).

Notice that plots, essential spreadsheets, etceteras are part of the "Results" section, and are thus placed *before* the Discussion when you assemble your report. For experiments that run over a two-week period, you will have two interleaved Experimental and Data workup sections. Appearance is still a factor in Lab Reports, so please write legibly, double-spaced, and if you make a lot of corrections in your calculations, write the final version out clearly on another page.

C. **REFERENCES:** As with the scientific article, it is unlikely that you designed the experiment on your own, referred to no textbooks, and used no literature data. Be sure to cite and give the complete reference for any handout and/or book that you used. You should have at least one reference to the source of a literature value for every experiment. References can be typed on a separate sheet or handwritten in your notebook.

D. **APPENDICES:** Useful raw data, excessive spreadsheet printouts, and other items that are not integral to understanding or interpreting your results should be included as appendices. Plots and spreadsheets that are essential to the explanation of the data analysis should be included in the body of the report (with your notebook pages). If there are many plots of the same type, include one in the body as an example, and the remainder as an appendix. Each appendix should contain a logical grouping of information, and be labeled with a letter and a title. Figures or tables within the appendix should be labeled A1, A2, or B1, B2 etc..

D. A Checklist for Effective Writing[5]

The following list is intended to help you in your revision process. After you have written a draft of your paper (or report), check through this list to see where you might need to start making changes. It may also be helpful to keep nearby as you are constructing the first draft.

Content:

Have you defined your subject?
Are the connections between your ideas clear?
Have you defined your scientific terms?
Have you anticipated questions that your readers are likely to ask?
Are your conclusions supported by evidence and logic?

Precision and Clarity

Did you use simple, specific words and sentences?
Have you used the correct words for your meaning (use a dictionary!!)?
Is your science correct (have you used numbers correctly, etc.)?
Did you provide details to support generalizations?

[5] Adapted from Moore, R. *Writing to Learn Science*, Saunders Publishing, Forth Worth (1997)

Will readers understand all of the pronouns that you have used?
Have you avoided jargon when possible?
Have you organized your thoughts logically?
Are all of the tables and figures necessary?
If so, are they well-designed, numbered, and titled?

Style and Reader's Expectations

Have you followed the subject as soon as possible with its verb?
Have you used a strong verb to express the action of every clause and sentence?
Have you put in the stress position the material that you want the reader to emphasize?
Have you put familiar information at the beginning of the sentence?
Have you ended your paragraphs with a topic, or summarizing, sentence?
Have you made smooth transitions between ideas?

Mechanics:

Have you removed dangling modifiers?
Are modifiers close to words that they modify?
Have you expressed similar ideas in similar ways?
Have you checked the spelling of all words?
Have you check punctuation?
Have you proofread a hard copy of your paper?
Have you asked a colleague to read your paper?

Some examples of what to avoid:

Below are some examples from a variety of student lab reports and from scientific papers that fail to convey the author's meaning. Think about how you might rewrite the sentences to be more clear, then be on the lookout for similar types of errors in your writing.

Watch out for scientific misstatements:

- The solvents were evaporated *in vacuo* at 40 °C under a stream of nitrogen.
- The inner molecules are resonating.
- The K_a can be calculated by using spectroscopy.
- The absorbance calculations were plotted.

Beware of dangling modifiers:

- After soaking in acid, I washed the glassware thoroughly.
- After killing the rat, the diet was tested.

Avoid separating related words:

- Here are some suggestions for handling the buffer problems from Sigma Chemical Company.

Beware of word order:

- We almost lost our entire sample.
- We lost almost our entire sample.

Beware of marooned pronouns:

- When we tried to follow the instructions on the package, we burned it.

Avoid expressing similar ideas in dissimilar ways:

- Einstein enjoyed physics, classical music, and to ride his bicycle.
- The limitations of this method are its limited sensitivity and that it is dependent on high humidity.

Avoid excessively general statements:

- VAGUE: The solutions were measured.

  SPECIFIC: The absorbances of the solutions were measured at 540 nm.