Chem 343 Lecture

How to write a good report

Feb 14, 2002
The objective of writing reports

1. To demonstrate the results of your experiments

2. To show your understanding of principles and data analysis of the experiments

3. To respond to lab assignments

4. To learn a good manner of formal scientific writing required for your future research activities.
A scientific paper is often organized in the following way:

- **Abstract** — A Short summary of the study
- **Introduction** — (1) Nature and scope of the study, (2) Review of the previous study (background), (3) Method used for the study, and (4) Principal results.
- **Materials and Methods** — Details of the experimental procedures Required to reproduce the results
- **Results** — (1) Overall description of the experiment (2) Data presented for the study (Spectra, measurements etc.)
- **Discussion** —
- **Acknowledgment** — Thanks to the persons who financially or scientifically helped your project
- **References**

In this class, the laboratory report for an experiment should consist of the following parts:

1) Title Page (1 page)
2) Abstract (1 page)
3) Introduction (1-3 pages)
4) Data and Calculations
5) Results
6) Discussion (3 pages)
7) Data Sheets and Spectra
8) References

The report would be 10-15 page long excluding spectra. You can add material and method or appendix if necessary.
1) Title Page

Put the lab title, your name, your e-mail address, your lab partner’s name, your TA’s name, and the date.

2) Abstracts

♠ An abstract is a brief statement (not more than a paragraph) of the study. It should include (1) the purpose of the study, (2) the method used, (3) main findings, (4) the principal conclusion.

♣ Quote actual values for one or two of your most important results. For example:

The rate constant for the reaction between x and y was determined spectrophotometrically by monitoring the absorption of product z at 500 nm as a function of distance in a flow tube. A value of \(0.82 \pm 0.02\) mol\(^{-1}\)s\(^{-1}\)L was obtained.

♣ Abstracts are written from objective viewpoints (see the above example) in most cases. Hence, the first person is rarely used in an abstract.

♣ Most of Abstract should be written in the past tense because it deals with the work already done.
3) Introduction

This is a description of the purpose and method of the experiment.

♠ A good Introduction generally keeps to the following rules: (1) presents the scope and nature of the study, (2) reviews the field of the study or related studies previously done, (3) states the method used, (4) indicates principal results, (5) indicates principal conclusion suggested by the results.

♣ Do not hold your most important finding until the last point of the report; Indicates it at Introduction. A scientific report should not be written as a detective story is.

♣ This should be written in your own words; Do not just copy the handout or other references.

♣ Do not include a diagram of the apparatus (include it in Material and Method section if requested).

♣ Do not include equations.
(4), (5) could be little confusing. For UV/VIS experiment I would write,

In this experiment, we will perform experimental UV/VIS spectroscopy of three polymetine dyes, A, B, and C as well as theoretical HMO calculation for the dyes. Comparison of these data will show how absorbed wave length and the energy between LUMO and HOMO are correlated.
4) Data and Calculations

♠ A summary of the data and calculations leading to the final results reported, along with the corresponding estimates of uncertainty.

All the essential items should appear in the body of the report, usually in tabular form, though in a few cases a plot of the raw data may be appropriate.

(i) Table

Quiz: What is wrong with this table?

Table 1. Volume dependence of the compressed air pressure

<table>
<thead>
<tr>
<th>Volume</th>
<th>Pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1.30000</td>
</tr>
<tr>
<td>5</td>
<td>2.20000</td>
</tr>
<tr>
<td>3</td>
<td>3.33333</td>
</tr>
<tr>
<td>2</td>
<td>5.10055</td>
</tr>
<tr>
<td>1</td>
<td>10.0333</td>
</tr>
</tbody>
</table>
Table 1. Volume dependence of the compressed air pressure

<table>
<thead>
<tr>
<th>Volume (mL)a)</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>5</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure (atm)b)</td>
<td>10.0±0.1</td>
<td>5.1±0.2</td>
<td>3.3±0.1</td>
<td>2.2±0.1</td>
<td>1.3±0.3</td>
</tr>
</tbody>
</table>

a) The error of the measurements was ±0.01 mL throughout the measurements.
b) The average of 5 measurements. The Lab works pressure sensor was used to measure the pressure. The errors were estimated from the standard deviations of the measurements.

♣ Units
♣ Uncertainty of measurements
♣ Number of digits
Quiz : What is wrong with the following calculation?

John obtained 4 pressure measurements 3.000, 3.206, 3.100, 3.142 atm. He rounded them off as 3, 3, 3, 3 and obtained the average of 3 atm with the error of 0 atm.

(ii) Calculation

♣ Consider carefully the number of digits carried in a calculation. Retain one or two doubtful digits. The question as to which digits are doubtful is determined from the estimated error. If you find after making the error estimates that you have carried unnecessary digits, you should round these off in the report.

♣ You can use average and standard deviation to estimate the appropriate number of digits.

\[ \langle x \rangle = (\Sigma x)/N \]
\[ \sigma_X = \left[ \Sigma(x - \langle x \rangle)^2/(N-1) \right]^{1/2} \]

Download about error analysis handout from the web page about the details.

♣ When multiple-step calculations are involved, it is helpful to make a table with results from each of the major steps in a different column.
(iii) Graph

Graphs must be generated by computer—Quattro Pro or any other program is acceptable (Excel is OK and installed at most PCs at the PChem Lab). However, please assume that your TAs are only familiar with Quattro Pro.
Quiz: Which graph is better? Mention three reasons.

Figure 1. Analysis of Labworks experiment.

Figure 1. Volume dependence of 1/P, where P is the pressure measured with Labworks pressure sensor.
5) Results

♠ Your final results should be collected together and presented along with the estimated uncertainties.

♣ The result section should be short and clear.

♣ Whenever possible, literature values should be given for comparison. Often the results and literature values can be placed in a single table.

♣ Important! Analyze your data immediately.

If your results are not as good as you think they should be, review the calculation—especially check numerical work, equations used, and units. If more experimental work is needed, it can be done during the later periods allotted to the experiment.
6) Discussion

♠ The discussion should include an evaluation of the quality of your data and an interpretation of the results. This is based partly on evidence within your own data and experience, theory, and partly on comparison of your results with literature values.

♣ When reviewing your own data, you should ask yourself whether the internal consistency is as good as it should be according to the error estimates made. Is there internal evidence of systematic error, for example, a much larger discrepancy between parallel runs than the apparent errors within each run? Are there unexpected trends in the data?

♣ Mention possible systematic errors and other factors which might contribute significantly to the error in the experiment but which were not allowed for in your quantitative error estimates. When possible, you should try to predict the directions of these errors. (For example, in measurement of heat of solution, incomplete dissolving of the sample will inevitably tend to give a low result.)

♣ If you have any hypothesis, prove it based on several independent data or comparison of your data with literature values.

♣ The discussion should be no more than 3 pages long.
7) References

All references, except the lab handout, should be explicitly cited. When information is obtained from a reference, that reference should be noted by a number in brackets in the text (i.e.,[l]). At the end of the report, the references are then given according to those numbers. See any page in a scientific journal for examples.

References of this lecture:
Format

♣ Your report should be computer generated
♣ Staple at the left shoulder
♣ Single space or double space (Ask your TA about his/her preference. I personally like double space.)
♣ 10-15 pages in single space (excluding spectra and datasheets)
♣ Have sufficient margin for TA's comments
♣ We appreciate larger fonts (12-14 point)
♣ Use good headings
Where to start

So we have to write a 10 page report with the following organization.

1) Title Page
2) Abstract
3) Introduction
4) Data and Calculations
5) Results
6) Discussion
7) Data Sheets and Spectra
8) References

Step 1.
It is a good idea to start with 4) Data and Calculations and 7) Data Sheets and Spectra, because without your data you cannot find anything to say. Also, it is easy to write this part.
**Step 2.** Analyze the result. If you need to do any experiments again, do so.

**Step 3.** Write a list of figures, tables, and spectra. Think about how to organize it.

For example.

Table 1. Waiting time $\tau$ dependence of the signal intensity $I(\tau)$.  
Figure 1. Plot of $I(\tau)$ vs $\tau$.  
Figure 2. Plot of $\log(I_0 - I(\tau))$ vs $\tau$ with linear least-square fitting

**Step 4.** Write up 5) Results based on a list obtained in Step 3. It is a good idea to think about the outline of 5) before you start.

For example,

5) Results

5.1) $^1$H and $^{13}$C chemical shifts of ethylbenzoate  
Table 5.1. $^1$H chemical shifts of ethylbenzoate  
Fig. 5.1. $^1$H NMR spectra of ethylbenzoate  
Table 5.2. $^{13}$C chemical shifts of ethylbenzoate  
Fig. 5.2. $^{13}$C NMR spectra of ethylbenzoate

5.2) $^{13}$C $T_1$ measurement of ethylbenzoate  
Fig. 5.3. Experimental scheme of this experiment  
Fig. 5.4. ??
Step 5. Go back to
1) Title Page
2) Abstract
3) Introduction
4) Data and Calculations
5) Results
6) Discussion
7) Data Sheets and Spectra
8) References

Prepare the overall outline. Especially, 3) and 6) must be well organized before you start writing.

Step 6. I prefer to finish writing in the order of 2) -> 6) -> 3) -> 8). However, it is up to you.

Grammar and Wording

• Refer to Reference [3] if you have any problems with grammar. It is a good book for general writing (and it is not so expensive.)
• Be aware that most of the readers of scientific papers and reports are English non-native.
• Formal style is preferred in scientific writing. Avoid slang.
Self check

Find out mistakes from the following sentences.

1) Neither oxygen nor nitrogen are noble gases.

2) The TA warned all the students not to mix 10 N NaOH and 5 N HCl, however, several students made the mistake because they did not go to pre-lab discussion.

3) Neglecting costs, Option A is the best choice because of its high thermal efficiency.

4) A series of measurements generally yield a more accurate final value.