Physical Chemistry Lab
Guidelines for Reports

Students will do the experiments in groups and may collaborate on graphs and calculations (indeed, I recommend checking calculations with lab partners) but every student must turn in his or her own report, the text of which should be original. Raw data, graphs, curve fits, and so on, may be the same among lab partners and may be shared or even photocopied. Reports should be typewritten. Equations, special symbols and superscripts and subscripts should be typewritten.

If text is copied from another source, be sure to cite the source. Do not copy sections of text from the instructions for the experiment. Your personal view and understanding is wanted, and that is best expressed in your own words.

Reports will vary depending on your tastes and the nature of each experiment or exercise. Every report should contain the following sections:

Title, names, date and abstract. These elements can go on the front page of the report. The abstract is a few sentences (typically 50-150 words) that identifies the experiment, describes the method or apparatus, and gives key results and important conclusions. Equations and references are not included in an abstract. Here is a sample cover page:

Luminescence of Fluorescein Mercury Acetate
by Yi Kumar

Physical Chemistry Laboratory CHEM 4644 Section 1
February 16, 2017
Lab partner: Rachel Xin

A sample of fluorescein mercury acetate was prepared in boric acid glass. Luminescence spectra were recorded with a Varian Cary Eclipse fluorescence spectrophotometer using an excitation wavelength of 420 nm. Steady-state emission maxima were observed at 470 nm and at 570 nm. Emission lifetimes were 1.0±0.4 and 3.0±0.6 seconds, respectively, at 25°C. The 570-nm emission was attributed to phosphorescence. Emission at 470 nm was interpreted as delayed fluorescence. The ratio of delayed fluorescence to phosphorescence intensity as a function of temperature, from 10°C to 70°C, yielded an activation energy for triplet-to-singlet back energy transfer of 36 ± 8 kJ/mol.

Here is how the journal Physical Review E describes abstracts:

The abstract should be self-contained (contain no footnotes). It should be adequate as an index (giving all subjects, major and minor, about which new information is given) and as a summary (giving the conclusions and all results of general interest in the article). It should be about 5% of the length of the article, but less than 500 words.

Introduction. Put the experiment into perspective for the reader. Write a short summary of the purpose of the experiment and the relationship of this experiment to the broader field of chemistry. Show important chemical reactions. Do not copy the introduction section of the lab instructions word-for-word. Use your own words.
Theory. Describe the background theory of the experiment. Define variables. State important mathematical equations, explaining what each equation means and will be used for. One could use a subset of the equations that appear in the lab instructions, picking the most important or most-used equations. Number equations near the right margin.

Experiments often include a related quantum-chemical calculation. If so, that should be described. Explain what was calculated and with what methods.

Experimental Method. Briefly describe the instruments, procedures and reagents used. Note important instrument settings. If the lab temperature is important, note that. Usually a few paragraphs suffice. If you departed from the instructions or if they are unclear, incomplete or wrong, describe those aspects of the procedure in detail. The methods section is ordinarily written in past tense. It is not written as instructions for another user, but rather is a record of what was done in the lab.

Results. Present your raw data in graphical or tabular form. Integrate graphs and tables with text, except that especially long tables may be attached following the references. If the experiment involved a spectrum, include the spectrum in your report.

Show sample calculations if the calculations, including units, are not obvious.

Present calculated and derived quantities, again in graphs or tables if appropriate. Tables should have headings (above tables), labels and units. Graphs need captions (below figures) with figure numbers. Mind significant figures.

Calculations often require linear fits through data. An example is the graph of the logarithm of a rate constant versus inverse temperature. When reporting the slope and intercept, also report the standard error (or confidence interval, if you prefer) in the slope and intercept.

Linear fits can be done with R or with a spreadsheet such as Excel.

From a linear model in R,

\[
\begin{align*}
> & \text{Ea; Ea.sigma;} \\
& [1] & 34.83584 & \text{kJ/mol} \\
> & \text{lnAlin; lnAlin.sigma;} \\
& [1] & 5.152699 & \text{kJ/mol}
\end{align*}
\]

#(ln(A) and its standard error)

\[
\begin{align*}
& [1] 17.00261 & \text{ /M/s} \\
& [1] 2.115331 & \text{ /M/s}
\end{align*}
\]

With 1-σ uncertainty, \(E_a=35\pm5 \text{ kJ/mol}\) and \(\ln(A)=17\pm2\), with \(A\) in \(\text{M}^{-1}\text{s}^{-1}\).

<table>
<thead>
<tr>
<th>Table 1. Regression statistics for Arrhenius plot from Excel.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Regression</td>
</tr>
<tr>
<td>Intercept</td>
</tr>
<tr>
<td>X Variable 1 (/K)</td>
</tr>
</tbody>
</table>

Figure 1. Arrhenius plot.
The regression report in Table 1 indicates, for example, that the slope equals $-4.2 \pm 1.2 \times 10^3 \text{K}$. I used $2\sigma (2\times0.6)$ as uncertainty. One could instead use $\sigma$ itself, or half of the confidence interval, $(5.8-2.6)/2 = 1.6$, as the uncertainty. Activation energy equals $-R$ times slope, so in this case $E_a = 35 \pm 10 \text{kJ/mol}$, where the "±10" is ±1.2 times $8.314 \text{J/mol·K}$.

**Discussion.** Summarize your final results (e.g., $\Delta H$, $pK$, $\nu_o$, $k_r$, $R_e$). Compare your results with literature values. You may find literature values in textbooks, handbooks, journals, or at authoritative web sites. The lab manual includes references to guide you to literature values. Cite your sources. When you refer to a literature value, indicate with a superscript number which reference contains the value. Comment on differences between experimental and theoretical or accepted results. Explain major differences or errors. Comment on the quality of your results and give any ideas you have for improving the experiment.

Explain the connection of your experimental result to a larger chemical issue. For example, if a rate coefficient was measured, is it fast or slow compared to other reactions, or is its temperature dependence normal or anomalous? If a vibration frequency was measured, is it typical of chemically similar bonds, or is it unusual? If resonance energy was measured, do the results support resonance as a real phenomenon?

**References.** Present a list of references that you cited in your report. Typically three or more references will be cited, including the lab instructions. Do not list all of the references given in the lab instructions unless you actually cite them. There are several different conventions for references. Here are examples following Chapter 14 of the *ACS Style Guide* (Anne Coghill and Lorrin Garson, Editors, American Chemical Society: Washington DC, 2006.):

General reference forms for journal articles and books:
Author1; Author2; Author3 *Journal* *Year*, *Volume*, *page*.
Author1; Author2; Author3 *Book Title*; Edition; Publisher: Place of Publication, *Year*;
*Volume Number*, *Pagination*.

A few examples:
Cave, R.J.; Newton, M.J. *J. Phys. Chem. A* 2014, 118(35), 7221-7234. **DOI:** 10.1021/jp408913k

For this course, you do not need to adhere rigidly to any particular reference format. Do be sure that references are clear, specific and complete.

To obtain full credit, include at least one outside reference to a source in the published literature. An outside reference is one that is not in the lab hand-out. Published literature includes journals and monographs and tables and even handbooks. Web sites are harder to evaluate. For example, the ChemBook site of the National Institutes of Standards and Technology is an excellent source, but Wikipedia is less reliable. Whatever its source, the outside reference should not merely appear in the reference list, it should also be cited in the report (e.g., in the introduction or in the discussion.)
Oral Reports

The oral report is in place of a written report. That is, if you give an oral report on an experiment then no written report is required for that experiment. Both (or three) students in the group are to prepare and present the report together.

The time and date of your oral report is on the lab schedule. An oral report should last about 15-20 minutes. Be prepared to answer questions about the experiment, calculations and results. Questions may be asked during and after your presentation.

Oral reports are almost always PowerPoint presentations. The projector in room 342 will project a computer presentation onto the whiteboard. A PC will be available. You may, if you prefer, use your own computer. You may use any mix of presentation software, the whiteboard and handouts to support your presentation.

Open with a title slide. Describe the experiment. Explain formulas you used. Show raw data. Show important sample calculations. Show your results in tables or graphs. Summarize and discuss your results. Compare your results to published results if possible. References may appear at the bottom of slides or may be collected at the end of the presentation.