Physical Chemistry Laboratory Reports

Investigations reported in the scientific literature are generally longer and have a more formal content than is required of the physical chemistry laboratory report (e. g., they do not answer a series of questions posed to them). In addition, they include a background review of previous related studies, have an expanded experimental section detailing the experimental setup and procedures used, and have an acknowledgment for those providing scientific or financial support. In this course it is assumed that the theory and procedure given in the experimental write-up apply and were followed. Thus, the laboratory report will have a somewhat more limited content.

The laboratory report will give the results of the experiment, show your understanding of the relevant principles involved, demonstrate your ability to analyze data, and provide the opportunity for you to learn how to report scientific results from your experiment in a literate and scientifically rigorous manner. As such, this course fulfills the “Writing-in-the-Discipline” graduation requirement of the College of Liberal Arts and Sciences. Excluding the Appendix, a typical report will be approximately ten to fifteen pages in length and should generally contain the following sections:

1) Title Page
2) Abstract
3) Introduction
4) Procedure
5) Data and Calculations
6) Results
7) Discussion
8) Answers to all Questions
9) Conclusions
10) References
11) Appendix
    - Copy of Original, Signed Data Sheets from your Notebook
    - Treatment of Experimental Data
    - Propagation of Errors
    - Printouts
    - Spectra

Reports must be typed on a word processor. Hand written reports will be rejected. The pages should be bound together with staples. Do not use covers or paper clips. The Chemistry

Department has a heavy duty stapler capable of stapling large numbers of pages. Including the above ten sections in a report does not guarantees a satisfactory physical chemistry laboratory report. The section on Data and Calculations should be clearly written and explained and all tables, figures, graphs, plots, printouts, spectra, indeed all of the ancillary material require a title and a sentence or more in the body of the report stating their relevance and significance. If they are not germane to any point you are attempting to make in your report do not include them (unless specifically requested to). By following the correct style in these sections, the reader should not have to form his or her own conclusions as the reader's conclusions should be that of the writer.

Title Page

The title page contains the full title of the laboratory experiment, your name, your lab partner's name, your TA's name, and the date.

Abstract

An abstract is limited to at most one paragraph on one page. It is a brief summary of the major purpose of the experiment, the method employed, the main findings / observations, and the principal conclusion (your interpretation). Quote actual values for one or two of the most important results. For example:

> The second order 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 ± 0.02 $L \cdot mol^{-1} \cdot s^{-1}$ was obtained at 298 K.

While more a matter of personal taste, abstracts can be written in the past tense as they refer to work which has already been done. However, the use of first person is avoided.

Introduction

This is a one- to three- page description of the scope and nature of the investigation, underlying theory, the method used, main results, and the principal conclusion derived from these results. This should be written in your own words: do not just copy the hand-out or other references. If a diagram of the experimental set-up is necessary it should be put in another section of the report entitled Experimental, not put in the Introduction.

Data and Calculations

This section summarizes how the data is employed in calculations leading to the final results reported, along with the corresponding estimates of uncertainties. It is imperative that this section be clearly written and all calculations transparent. Thus, each equation must be given with a sample calculation. Justify and explain your calculations.

All the essential items should appear together, usually in tabular form, though in some cases a plot of the raw data may be appropriate. Each item in a table should be accompanied by units and an estimate of uncertainty. If the errors are the same for all entries in one column, the estimate can be placed at the head of the column or with the first entry. Otherwise, errors should be given for several cases to illustrate the variation. 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.

One sample illustration for each type of non-trivial calculation should be shown. For each type of calculation, give the equation, define the symbols used, show substitutions, and report the calculated result accompanied by units and an estimate of experimental error. The sample illustration should also show how the error was calculated (propagation of errors). Arithmetic details should be omitted. Minor data handling steps (such as subtractions of weighings or burette readings) should be carried out on the data sheets in your laboratory notebook and a copy placed in the Appendix.

The estimate of the uncertainty of a measurement (called the standard deviation σ) is obtained by assessing the limitations of the equipment used and/or by repetitive measurement. For example a thermometer graduated in degrees can usually be read to the nearest 0.2° to 0.5° and the volume of liquid contained in a 50-mL burette can typically be estimated to the nearest 0.02 mL. For a repetitive measurement, the average value and its standard deviation can readily be calculated.

Once reliable estimates of the uncertainties associated with each of the individual measurements have been made, their combined effect on the value to be reported must be assessed by propagation of errors. For instance, say that one wishes to report a value for the pressure for one mole of a gas, assumed to be ideal, based upon experimental measurements of the temperature and volume of the gas. One measures the temperature T and has an estimate for its uncertainty, σ_T, and similarly for the volume measurement, V and σ_V. Using the idea gas equation of state one propagates the errors in temperature and volume to obtain the error in pressure, given by the standard deviation σ_P. In terms of the variance, the propagated error is:

$$\sigma_P = \sqrt{\left(\frac{\partial P}{\partial T}\right)_V^2 \cdot \sigma_T^2 + \left(\frac{\partial P}{\partial V}\right)_T^2 \cdot \sigma_V^2}$$

One would then report the value for the pressure given by the ideal gas equation of state and calculated using the experimentally determined temperature and volume. The reported uncertainty in this number would be the square root of the above variance. More discussion on standard deviations and propagations of error can be found in the handout “Uncertainty in Measurement.”

When significant figures are properly employed, standard deviations often have one more decimal place than the measurement (or average value) to which they correspond. Here are two examples:

m = 11.5 σ_M = 0.69 and b = -21.63, σ_b = 0.027

While it is tempting to round the above two error estimates to 0.7 and 0.03, respectively, so that the number itself and its estimated error would have the same number of decimal places, such a procedure can lead to an erroneous error estimate especially if these errors are to be propagated. Only round off a number and its corresponding error estimate to the same number of decimal places when this number is the final result to be reported.

Graphs must be generated by computer- MATLAB, Excel, Sigmaplot, Quattro Pro or any other program is acceptable. MATLAB, Excel and Sigmaplot are available on the computers in 2013A SEL When a linear relationship is anticipated, the method of linear least squares should be used to find the “best” straight line that can be drawn through the set of (x, y) data points. The equation for the line determined by the least squares method should be given (i.e., the slope and intercept). The calculated line should be shown on a plot along with each original data point. The quality of the fit is shown by giving the correlation coefficient (R^2), standard deviation of the fit (standard deviation of the regression), standard deviation of the slope, and standard deviation of the intercept. Most linear regression fitting programs give these four measures or criteria for reporting the quality of the fit. We also have an example of an Excel spreadsheet on the web site which calculates these values.

A nonlinear regression analysis is used when the relationship between a set of (x, y) data points is not linear. Statistical or scientific spreadsheets can do this analysis (e. g., Solver in Excel, fminsearch in MATLAB) as well as built-in regression programs on your calculator (as on the TI-86). For a nonlinear regression, the equation determined by the analysis should be given along with all the regression parameters. Again, the calculated line should be shown on a plot along with each original data point. The quality of the lit is shown by the standard deviation of the fit and the standard deviation of each regression parameter.

Results

The final results of the laboratory report should be collected together and clearly presented along with the estimated uncertainties. Be sure that the results have the proper number of significant figures and the appropriate units. Whenever possible, literature values should be given for comparison. Always site the source of the literature values. Often the final results and literature values can be placed in a single table for ready comparison. Literature values can be found in standard references available in the SES Science Library.

If the results are not as good as you think they should be, review the calculations (especially check numerical work), the equations used, and the units. Do this review as early as possible so that if more experimental work is needed, it can be done during the later periods allotted to the experiment. Errors in calculation are common and generally inexcusable. If you are uncertain about some part of the calculation, consult a TA or faculty member and try to be sure the calculations are correct before completing the report. If the fault lies in the data, you are strongly urged to repeat some of the measurements.

Discussion

The discussion should generally not exceed three pages. It should include an interpretation of the results and an evaluation of the quality of the data. This is based partly on evidence within your own data and experience, and partly on comparison of your results with literature values. When reviewing your data, ask yourself whether the internal consistency is as good as it should be according to the error estimates made. Is there evidence of a 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?

When comparing with literature values, do your results agree as well as should be expected from your quantitative error estimates? If not, do you see evidence of systematic error - for example, are your points consistently low or high? Are there clear trends in the errors? In any case, you should mention possible systematic errors and other factors which might contribute significantly to the error in the experiment but which were not accounted for in the quantitative error estimates. When possible, try to predict the directions of these errors. (For example, in measurement of the heat of solution, incomplete dissolving of the sample will inevitably tend to give a low result.)

Answers to all Questions

Unless told to include in another section of the laboratory report, give the answer to all questions posed in the lab write-up and any other handouts.

Conclusions

A brief statement about purpose of experiment, results, errors, problems, with an emphasis upon your interpretation of your results.

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., [1]). At the end of the report, the references are given according to those numbers. See any page in a scientific journal for examples.

Points to Remember

- use scientific reporting methods:
  - SI units
  - significant figures
  - standard deviations
  - error propagations
  - least squares/regression analyses
- check for all tables, figures, graphs, plots, spectra, and appendices:
  - titled and numbered
  - entries labeled or otherwise unambiguously identified

- discussed in body of report
- figures, graphs, and plots at least one half of a page large

include in Data and Calculations section:

- relevant formulas
- sample calculations
- error propagations

include in Results section:

- final results with estimated uncertainty
- comparison to literature values

include in Discussion section:

- interpretation of results
- evaluation of data quality
- lucid error analysis

read over report for the quality of your writing:

- clarity
- organization
- spelling
- grammar
- punctuation
- first person references (omit)