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Instructions for writing reports in physical chemistry laboratory

The report should contain the following parts:

1. **Title**
   Title of the experiment, your name and email address, date

2. **Abstract**
   An abstract is a brief statement (not more than a paragraph) of the results of the experiment and the method used. 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 distance in a flow tube. A value of (0.82 + 0.02) L $mol^{-1}s^{-1}$ was obtained.

3. **Introduction (1-2 pages)**
   This is a description of the purpose and the method of the experiment. In this section also a basic principle of the phenomenon should be explained. For example, it may be a brief description about fluorescence spectroscopy. You may explain what kind of information you may get from the molecules with this method. What is the basic principle of the measurement?

4. **Results**
   This section includes 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. Each item should be accompanied by units and an estimate of uncertainty. Only minor reductions (such as subtractions of weightings or burette readings) should be carried out on the data sheet.

   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, state the equation, define the symbols used, show substitutions, and give the calculated result accompanied by units and an estimate of experimental error. The sample should also show how the error was calculated. Arithmetic details should be omitted.

For function $q = q(x,\ldots,z)$ the error can be estimated with the propagation of error method, when the errors $\delta x,\ldots,\delta z$ for the variables $x,\ldots,z$ are known and they are independent and random. The error for function q can be thus calculated

$$\delta q = \sqrt{\left(\frac{\partial q}{\partial x}\delta x\right)^2 + \ldots + \left(\frac{\partial q}{\partial z}\delta z\right)^2} \qquad (1)$$

For example the error for the calculated density 1,067 g/cm^3 *($\rho=m/V$) from the measured values m=* 21,34±0.01 g *and V=20,00*± 0,12 cm^3 *is calculated from the following function*

$$\delta\rho = \sqrt{\left(\frac{\partial\rho}{\partial m}\delta m\right)^2 + \left(\frac{\partial\rho}{\partial V}\delta V\right)^2} \qquad (2)$$

The partial derivatives for equation (2) can be calculated to give

$$\frac{\partial\rho}{\partial m} = \frac{1}{V}\times 1 = \frac{1}{V} \qquad (3)$$

$$\frac{\partial\rho}{\partial V} = m\times(-1\cdot V^{-2}) = -\frac{m}{V^2} \qquad (4)$$

and are substituted to the equation (2)

$$\delta\rho = \sqrt{\left(\frac{1}{V}\delta m\right)^2 + \left(-\frac{m}{V^2}\delta V\right)^2} \qquad (4)$$

Now the error for the density can be calculated

$$\delta\rho = \sqrt{\left(\frac{1}{20,00}\cdot 0,01\right)^2 + \left(-\frac{21,34}{(20,00)^2}\cdot 0,12\right)^2} = 0,00642\left(\frac{g}{cm^3}\right) \qquad (5)$$

and thus the final result is

ρ= 1,067 ± 0,007 g/cm3.

Consider carefully the number of digits carried in a calculation. You must be sure to carry enough digits to preserve the accuracy of the data. On the other hand, it only wastes effort and increases chances for error to carry many meaningless digits. A good rule is to 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. Estimates of experimental error should be attached to the various table entries. If the error is practically 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 so as to illustrate the variation. Error estimates should be rounded off to one or at most two digits.

The error is given with an accuracy of one digit except when error is smaller than 15 units. Then error is given with an accuracy of two digits. The errors are always rounded upwards.

For example:

- if the number is 32.21367 and its error is 2,34 the result should be given as 32±3

- If the error would be smaller like 0.124 then the result would be 32.21±0.13

The number itself and the estimated error should be rounded off consistently (e.g. 32.14 ±0.05)

It is recommended to use some computer program (eg. excel, origin) for making graphs of you data. Include title of the figure and axis titles in the figure. If you have fitted the data by using some function (eg. Linear regression or exponential growth) include also the equation with the parameters of the best fit. Notice that when you use a computer program for fitting your data the program gives you also the errors for example for the slope and the intercept in the case of linear regression.

5. Discussion

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

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? Comparing with the literature data, do you find that 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 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.) In some cases, you will need to consider the calculation carefully in order to predict the direction of an effect on the final results.

6. **References**
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.

7. **Appendix**
Attach your laboratory notes, big tables (if any) *etc*. as separate sheets in the end of the report.