# Background Notes I: Analysis of Experimental Data 

## Introduction

Scientists work according to what is known as the "scientific method". This consists of four steps:
(a) First we observe an interesting or unusual phenomenon;
(b) A possible explanation (a hypothesis) to explain the observation is devised;
(c) Experiments are (i) designed, and (ii) performed to test the hypothesis; and
(d) The results of the experiment are checked to determine whether they lend support to the hypothesis.

In the sort of work which you will do as part of your degree course, most experimental work in physical chemistry relates to step (c ii) and to (d). Normally both the topic to be studied (for example, the enthalpy of combustion of some organic chemical) and the relevant background theory (in this case, classical thermodynamics) are well known. You make the relevant physical measurements, and check that the results are in accord with theory.

Design of hypotheses (step b), and of experiments (ci) is an important aspect of Part II research, and you may encounter examples of it later in the PTCL practical course.

If an experiment is to be effective, it must be able to discriminate between the predictions of competing theories. This is less simple than it may sound since it requires that you be able to estimate the "quality" of your results. A simple example will help to explain this point.

Suppose you were trying to identify a gas. It's at low pressure, so might be a gas or a liquid at room temperature. Since you have a mass spectrometer you decide to use it to determine the molecular mass of the gas. The result is 43.9 Daltons. Is this sufficient to identify the gas?

The answer is ..... probably. But first you need to know how accurate the measurement is.

In almost every measurement there is some uncertainty. If you measure the height of a friend, you might perhaps quote the result to $\pm 1 \mathrm{~cm}$, or even (if you were unreasonably optimistic!) to $\pm 0.1 \mathrm{~cm}$. The " $\pm$ " bit is the "error" in your measurement. It is important to realise that in this context, error means "uncertainty" - the term does not imply that you have made a mistake in measurement (though of course that might have happened), merely that you cannot specify the result of the measurement absolutely precisely.

The size of the experimental error dictates how you can interpret the results from your experiment. Suppose you estimate that the mass spectrometry measurement had an error of $\pm 1.5$. Your result must now be shown as $43.9 \pm 1.5$ Daltons, so the gas you are trying to identify could be any compound whose molecular mass lies between 42.4 and 45.4.

Several compounds are now possible, including carbon dioxide (molecular weight of 44.01), propane (44.07), ethyl alcohol (45.06) or ethylamine (45.09) If the uncertainty was a bit larger, other possibilities, such as argon, would also exist. By contrast, if the error were just $\pm 0.15$, all but carbon dioxide would be ruled out. You can see, therefore, that merely quoting the result of an experiment is not sufficient - you must always include the probable uncertainty. In fact, the results you calculate at the end of an experiment are virtually useless without an estimate of their quality.

Estimation of the reliability of your data is a vital task in science, and these notes, together with experiments X2 and X3, are concerned largely with the task of handling experimental error. In a sense, measurements are the "products" of physical chemistry in the same way that samples are the products of an organic laboratory exercise. Just as you might use NMR or IR spectroscopy to determine the purity of a compound you had prepared in an organic lab, so you must assess the quality of the data you extract from a physical experiment through an analysis of error.

You must therefore learn how to determine the magnitude of the error associated with your data. Demonstrators will expect you to apply the methods of analysis discussed in these notes to every experiment you carry out in the PTCL.

## 1

## Accuracy and precision

We'll start with two terms which are frequently confused: accuracy and precision.

- The accuracy of a result indicates how close it is to the theoretical value.
- The precision is a measure of how similar are repeated measurements of the same property.

while those of $B$ are precise but not very accurate. C's shots are both precise and accurate.

Thus an accurate measurement agrees well with the actual ("true") value, while a precise measurement is reproducible from one measurement to the next. Precise measurements are not necessarily accurate, therefore, although accurate ones are necessarily precise.

The figure to the left shows the results when three people fired at a target. A's shots are neither accurate nor precise,

## 2 Random and systematic errors

Experimental errors are unavoidable. They can be divided into two categories.
-Systematic errors might be due to faulty calibration, limitations in the theory underlying an experiment, sample contamination or instrument drift; they give rise to a uniform and reproducible error in every reading of the same type.
-Random errors are due to inaccuracies in the process of measurement, and are unpredictable. Random errors prevent measurements from being identical and arise from random fluctuations in factors such as temperature or electrical noise, or simply from the inability of the experimenter to read a measuring instrument in precisely the same way each time.

In the figure on the right a number of measurements have been made and plotted as a histogram. The average value
 of the measurements is close to 15 . If 15 is the "correct" value, then the measurements show a roughly random (Gaussian) scatter around the mean. If, on the other hand, the correct value is 23 , then the measurements show not just a random scatter, but evidently the whole set of measurements is shifted, and this suggests some kind of systematic error in the data.

In these notes we will present a little of the mathematics of random errors, and, through exercises, show the practical implications of the presence of error in data.

You might think that systematic errors would be easy to spot, but often they are harder to detect than random errors (essentially because we may not know what the "right" answer is, so it is hard to tell whether the final result is close to it or not). A characteristic indication of their presence is if significantly different results are obtained when the same physical quantity is measured using two different methods. A famous example is the discrepancy in values of the charge on the electron between Millikan's oil drop experiment and the ratio of the Faraday to Avogadro's constant, which was ultimately traced to an incorrect value of the viscosity of air from which the radius of the drop was deduced.

## 3 Two comments on systematic error

(a) The origin of the error has no bearing on the precision of the result. If the weight of a sample is $25.0049 \pm 0.0004 \mathrm{~g}$, the precision is not a function of the type of error.
(b) Random errors are unavoidable and will arise in any experiment. However, they can be handled using statistics and their effect may be diminished by repeating the experiment many times. Systematic errors, on the other hand, cannot always be allowed for. This is because

- although we may know of (or guess) the existence of a systematic error, we may be unable to determine its size; or
- we may not even know that a systematic error is affecting our measurements.

It is important to realise that systematic errors are not occasional irritations, but a complication present in almost every experiment. If you perform a titration, the calibration of the burette will be correct only to within certain limits; thus all your titration volumes are probably too small or too large. Mechanical balances may deteriorate with use - they can be read to the same precision as when they were new, yet every reading may be faulty by the same amount.

In many experiments the theory on which the experiment is based will contain approximations (for example, you may assume ideal gas behaviour, which may be appropriate under the conditions of the experiment for hydrogen, but not for carbon dioxide). Every result may be slightly wrong as a result. Furthermore, the extent of the error may depend upon experimental conditions. For example, deviations from ideal gas behaviour generally become more pronounced as the pressure increases.

It is often difficult to identify systematic errors and to estimate their magnitude. This is no way means that they can be ignored. Indeed, systematic errors are a more serious
obstacle to the collection of reliable data than are random errors, since the latter can be allowed for mathematically.

## 4

## How to analyse random error

Repeated measurements of the same quantity usually contain random error. If the error is random, its size is determined by 'chance' and readings will cluster about the mean value, showing a 'normal' or Gaussian distribution. Random errors are completely unpredictable - and unavoidable. They cannot be eliminated by repeating the experiment very carefully, but their effect may be reduced by performing the experiment many times and treating the results statistically. If sufficient readings are available, (usually six is a realistic minimum), we can analyse those readings to determine the average (mean) of the readings, and the chance that the true value of the reading lies within a certain tolerance of that mean.

This analysis is straightforward and should always be carried out when random error has produced significant scatter in your experimental results. It is generally very easy to do using a standard calculator.

The treatment of random errors starts from the assumption that the true value, or mean, $m$, of any quantity $x$ can be measured only within a tolerance or standard deviation, s, such that the probability $P(x) d x$ of obtaining a value between $x$ and $x+d x$ follows the normal distribution.

The function $P(x)$ takes the mathematical form:

$$
\begin{equation*}
P(x)=\left(2 \pi \sigma^{2}\right)^{\frac{1}{2}} \exp \left[-(x-\mu)^{2} / 2 \sigma^{2}\right] \tag{1}
\end{equation*}
$$

which has the property that $67 \%$ of an infinite sample of readings of $x$ lie within the range $\mu \pm \sigma, 95 \%$ lie within $\mu \pm 2 \sigma$, and $99 \%$ within $3 \sigma$ of the mean.

Section 5 below explains how to find the mean and standard deviation of a set of measurements, and section 6 deals with comparisons between different experiments. The fitting of straight line graphs is covered in section 7. Finally section 8 shows how errors in measured quantities, $x$ and $y$ for example, combine to yield the error in some function $z=f(x, y)$ of physical interest ("Propagation of errors").

## 5 Estimates of the mean and standard deviation

It is a simple matter to calculate the mean and standard deviation from a set of measurements. Given a set of independent readings $x_{1}, x_{2}, \ldots x_{n}$, the mean and standard deviation are given respectively by:

$$
\begin{align*}
& \bar{x}=\frac{1}{n}\left(x_{1}+x_{2}+\ldots+x_{n}\right)=\frac{1}{n} \sum_{i=1}^{n} x_{i}  \tag{2}\\
& \sigma^{2}=\frac{1}{n-1} \sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2} \tag{3}
\end{align*}
$$

The factor $(n-1)^{-1}$ in equation 3 arises because only $(n-1)$ of the $\left\{x_{i}\right\}$ are independent once their average is specified. The estimated standard deviation, $\sigma$ relates to a single measurement of $x$. Results should be reported as

$$
\begin{equation*}
x=\bar{x} \pm \sigma / \sqrt{n} \tag{4}
\end{equation*}
$$

Example: Suppose you measured the frequency of vibration of the $C-O$ bond in carbon monoxide several times and found the values $2140,2145,2139,2150,2146,2142,2144 \mathrm{~cm}^{-1}$, you would report the final mean value for the frequency as $2143.7 \pm 1.4 \mathrm{~cm}^{-1}$, since the standard deviation, $\sigma$, equals 3.8. (The odd looking units, $\mathrm{cm}^{-1}$, are called "wavenumbers", and are a unit of energy which you will encounter in 2nd year).

## 6 Comparison of results from different experiments

Often measurements are made of a property for which reliable values have already been determined. It is then important to know how to compare your own results with those from other workers. The simplest situation is when you wish to compare your mean reading with a literature value, or theoretical prediction, $\mu$, when you have made a large number of readings, say 25 or more Provided that the only significant error is random, the estimated mean may then be assumed to be derived from a normal distribution, such that there is a $95 \%$ confidence that it lies within $2 \sigma / \mathrm{n}^{1 / 2}$ of its true value. Hence if

$$
\begin{equation*}
|\bar{x}-\mu| \geqq 2 \sigma / \sqrt{n} \tag{5}
\end{equation*}
$$

there is "a significant difference between the two values at the $95 \%$ level" (This means that there is a $95 \%$ chance that the two values are genuinely different, rather than any difference arising purely from random scatter about a common mean).

## 7 Straight line graphs

Plotting a 'best' straight line through a set of points is one of the commonest tasks in data analysis. It is generally recognised that this line minimises the sum of the squared deviations of the ordinates of the experimental points from the line. This is a useful assumption, provided that the error in the abscissa is negligible compared to that in the ordinate, which will often be the case. The line calculated by Least Squares Analysis will only be the 'best' mathematically when the experimental errors are Gaussian in distribution.

A least squares line should be fitted through data in which the dependent and independent variables are thought to bear a linear relationship, even if you are not sure
the experimental errors are Gaussian. However, this fit is only likely to be reliable when you have more than three points (preferably at least six). If the uncertainty in both variables is similar in magnitude, a full least squares procedure should be used (York, Can. J. Phys., 44, 1079, 1966).

For the common situation in which the $x$-coordinate is assumed free of error, the fit can conveniently be accomplished by using a spreadsheet or calculator. We outline the mathematics that underlie this method below.

A least squares analysis should not be regarded as a substitute for drawing a graph, since a least squares line can be calculated for any set of points, even four points lying almost in a square. A plot of your experimental data will show information that the least squares calculation on its own will not reveal. For example: perhaps your "straight" line is actually curved. If it is, the curvature might suggest some limitation in the
 theory behind the experiment, or that some systematic error exists in the measurements. Does the scatter increase along the line? If so, are later results less reliable? A least squares fit might give a good correlation coefficient, indicating a good straight line, but would not tell you if scatter is constant - a graph is needed to show this.

The choice of a 'best' straight line through a set of points $\left(x_{1}, y_{1}\right),\left(x_{2}, y_{2}\right), \ldots . .\left(x_{n}, y_{n}\right)$ depends upon the relative proportional errors in the $\left\{x_{i}\right\}$ and $\left\{y_{i}\right\}$. The simplest situation occurs when the $\left\{x_{i}\right\}$ are precisely known, in which case the line is taken as

$$
\begin{equation*}
y=m x+c \tag{6}
\end{equation*}
$$

with $m$ and $c$ chosen to minimise the sum of discrepancies between the measured values $y_{i}$ and the predictions ( $m x_{i}+c$ ). In other words, $m$ and $c$ are determined by the equation

$$
\begin{equation*}
(\delta F / \delta m)=(\delta F / \delta c)=0 \tag{7}
\end{equation*}
$$

where $F(m, c)$ is the sum of the squared discrepancies

$$
\begin{equation*}
F(m, x)=\sum_{i=1}^{n}\left(y_{i}-m x_{i}-c\right)^{2} \tag{8}
\end{equation*}
$$

One finds after some manipulation that the 'best' estimates of $m$ and $c$ may be expressed as:

$$
\begin{align*}
& m=S(x, y) /[S(x)]^{2}  \tag{9}\\
& c=\bar{y}-m \bar{x} \tag{10}
\end{align*}
$$

where

$$
\begin{align*}
& {[S(x)]^{2}=\frac{1}{n} \sum\left(x_{i}-\bar{x}\right)^{2}=\left(\frac{1}{n} \sum x_{i}^{2}\right)-\bar{x}^{2}}  \tag{11}\\
& {[S(y)]^{2}=\frac{1}{n} \sum\left(y_{i}-\bar{y}\right)^{2}=\left(\frac{1}{n} \sum y_{i}^{2}\right)-\bar{y}^{2}}  \tag{12}\\
& S(x, y)=\frac{1}{n} \sum\left(x_{i}-\bar{x}\right)\left(y_{i}-\bar{y}\right)
\end{align*}
$$

Turning to the estimate of error, the first step is to test the validity of the linear assumption embodied in the equations above by calculating the correlation coefficient. This is often quoted after a least squares analysis. It gives a value between -1 and +1 which shows how well the data approximate to a straight line (a value of 1 indicates a perfect correlation, while a purely random scatter, with no correlation between $x$ and $y$, yields $r=0$ ).

Although correlation coefficients are widely used in the social sciences, they are of only limited value in the sort of fit you will perform, since for any reasonable set of chemical data from an undergraduate experiment, the correlation coefficient will be $>0.9$ (and often >0.99). It thus often provides little guidance in deciding whether or not the data gathered during an (undergraduate) experiment are reliable.

$$
\begin{equation*}
r=S(x, y) /[S(x) S(y)] \tag{13}
\end{equation*}
$$

## 8 Propagation of errors (combining errors)

Sometimes, the final result of an experiment is a quantity you have measured directly. The error is then just the error in the measurement itself. More often, however, intermediate results are combined in a number of mathematical steps to give a final result. The question then arises: how should the errors in the individual measurements be combined to yield an estimate of the error in the final result?

The most direct way to proceed would be to insert the measurements with their error bounds into the formula which defines your result and work out an answer, which will then have the correct error bound. However, this method is a bit tedious, and it is useful to know how this can be done with a minimum of difficulty through calculus.

This section concerns the magnitude of error in a function $f(x)$ of physical interest implied by an estimated error in the measured variable $x$. More generally, errors in several measured quantities $x, y, z \ldots$ might accumulate to give errors in the function $f(x$, $y, z, \ldots$ ) of interest. In the single variable case

$$
\begin{equation*}
\delta f=\left|f\left(x+\frac{\delta x}{2}\right)-f\left(x-\frac{\delta x}{2}\right)\right| \tag{14}
\end{equation*}
$$

In other words, the required error is simply the change in $f(x)$ between the highest and lowest values of $x$ in the range $x \pm \delta x / 2$. In cases where $f(x)$ shows perceptible curvature over the range, this is the most reliable procedure.

Commonly, however, the error in $x$ may be assumed to be sufficiently small that the linear approximation

$$
\begin{equation*}
f(x)=f(x)+f^{\prime}(x)(x-\bar{x}) \tag{15}
\end{equation*}
$$

is valid over the range $x \pm \delta x / 2$. In this case, equation 14 goes over to

$$
\begin{equation*}
\delta f=\left|f^{\prime}(x)\right| \delta x \tag{16}
\end{equation*}
$$

For example, the radioactive decay constant $k$ is related to the half-life $t$ of a radioactive species by the equation

$$
\begin{equation*}
k=\ln 2 / t \tag{17}
\end{equation*}
$$

from which the uncertainty in $k$ arising from an uncertainty $d t$ is given by

$$
\begin{equation*}
\delta k=\left|\frac{d k}{d t}\right| \delta t=\left(\ln 2 / t^{2}\right) d t \tag{18}
\end{equation*}
$$

subject to the requirement that

$$
\begin{equation*}
\left|\frac{d^{2} k}{d t^{2}}\right| \delta t \ll\left(\frac{d k}{d t}\right) \text { or } 2(\delta t / t) \ll 1 \tag{19}
\end{equation*}
$$

The generalisation of equation 16 to a function of several variables involves extending equation 15 to the form

$$
\begin{equation*}
f(x, y, \ldots)=f(x, y, \ldots .)+\frac{\partial f}{\partial x}(x-\bar{x})+\frac{\partial f}{\partial y}(y-\bar{y})+\ldots \tag{20}
\end{equation*}
$$

Provided that the measured quantities $x, y, \ldots$ are independent variables, the error in $f$ is given by

$$
\begin{equation*}
(\delta f)^{2}=\left(\frac{\partial f}{\partial x}\right)^{2}(\delta x)^{2}+\left(\frac{\partial f}{\partial y}\right)^{2}(\delta y)^{2}+\ldots \tag{21}
\end{equation*}
$$

## 9 "Instrument error"

Frequently, you will not have enough repeat measurements to be able to reliably calculate a standard deviation. For example, you might have performed a series of titrations at different stages in an experiment, so that the same solution was never analysed twice. In such a case, the error may be estimated by assessing the precision of each reading.

A standard burette is calibrated at $0.1 \mathrm{~cm}^{3}$ intervals. By eye, a careful observer might be able to estimate the volume in the burette to $0.01 \mathrm{~cm}^{3}$, thus the error in the volume delivered would be $0.02 \mathrm{~cm}^{3}$ ( $0.01 \mathrm{~cm}^{3}$ at both the start and finish of the titration). In
the absence of repeated measurements, this should be given as the error in the measured volume.

## 10 Be Realistic when Assessing Errors

Despite what you read above about the error in titrant volume being about $0.02 \mathrm{~cm}^{3}$, you must remember that the error is determined by you; it is not some number to be stuck on your results because someone told you what it was. Not every student will have the skill required to perform a titration to such precision. The error you quote must be an honest reflection of how precise you think your own measurements are.

## 11 Significant Figures

The sun is $93,000,000$ miles from the Earth. What does that mean? Does it, for example, mean that the distance is $93,000,000$ miles and not $92,999,999$ or $93,000,001$ miles? Obviously not. What is meant is that the (average) distance is closer to 93 million miles than to 92 or 94 million miles. To make this clearer, we generally would write this as $9.3 \times 10^{7}$ miles, showing only two significant figures.

Leading or trailing zeros may be confusing and are best eliminated by using 'scientific notation'. If the number 2.1 were stated as 2.10 (i.e. to three significant figures), the 0 would be taken as conveying meaning - in other words, we were sure that the value was closer to 2.10 than to 2.09 or 2.11 .

## 12 Rounding

Suppose the average of a number of titrations is $25.02749 \mathrm{~cm}^{3}$. Calculation has yielded this figure, but what should be quoted in a report? Values given at the end of a calculation should be rounded so that only significant figures are shown. We have seen earlier that the error in titration when carried out by a competent experimentalist should be about $0.02 \mathrm{~cm}^{3}$, so that the average titrant volume should be rounded to two decimal places and shown as $25.03 \pm 0.02 \mathrm{~cm}^{3}$. If you have a sufficiently large number of readings, you should calculate and quote the standard deviation for the data.

Do not quote significant figures beyond the figure at which the error is likely to occur.

## 13 Non-linear Fitting

On occasion, your data may lie along a curve, rather than a straight line. A least-squares fit is still appropriate, though the mathematics required to fit a polynomial is somewhat
more tricky. Most calculators will perform such a fit, but you should not use a larger degree of polynomial than seems justified.

## 14 Presentation of Graphs

Whenever your results show trends, the information should be shown in the form of tables and/or graphs. When plotting graphs, make note of - and use - the following conventions:
-The independent variable (the variable which causes the change plotted) is shown as the abscissa ( $x$-axis) and the dependent variable as the ordinate ( $y$-axis).
-Data points must be shown clearly. Do not merely use dots, which will be lost if the line passes through them. Open points (dots with a small circle drawn round) are simple and clear.

- If more than one set of data is to appear on the same graph, use different symbols for each set. In such cases show on the graph the relationship between the data and the symbols used.
- Draw the fitted line up to each data point, rather than through it, so that each point remains clearly visible.
-Estimates of the error in each point should, when larger than the symbol used for the point, be indicated by error bars. An error bar is a small bar drawn through a point, showing the extreme limits of the possible value for the point. For example, if an experimental point is $(4,25.17 \pm 0.1)$, a point should be plotted at $(4,25.17)$, and an error bar drawn from $(4,25.07)$ to $(4,25.27)$. If a data point contains error in the $x$-coordinate, error bars should be drawn in the direction of this axis also.
- Axes must be labelled with their identity and units. The graph should carry a clear legend, but not lengthy explanation.
-Each division on your graph paper should represent some simple number of units, such as 100 s or 1 kg . Do not divide your graph paper into units of 13.9 furlongs or 11 grains per cubit.
- When drawing lines of maximum and minimum slope through your data points, every data point should be no further away from the lines of maximum and minimum slope than the furthest point is away from the 'best fit' line.

The uncertainty of the slope or intercept of a graph is judged by drawing extreme line fits to the points. These lines are not lines of the greatest and smallest possible slope which can be drawn through some selected pair of data points. Instead, maximum and
minimum lines represent the outer limits for a best fit line - they should themselves be reasonable fits to the data.

## 15 Units and Symbols

The International System of Units (SI) is used widely in science and should be used throughout your own work. Numerical results in your reports (including graphs and tables) should always clearly show the relevant units. The seven basic units are:

| Physical quantity | Name of SI <br> unit | Symbol |
| :--- | :---: | :---: |
| Length | metre | m |
| Mass | kilogram | kg |
| Time | second | s |
| Electric current | ampere | A |
| Temperature | Kelvin | K |
| Luminous intensity | candela | cd |
| Amount of substance | mole | mol |

It is possible to express all other quantities in terms of these units (see table below).

| Physical quantity | SI Unit | Symbol | Definition |
| :--- | :--- | :---: | :--- |
| Energy | Joule | J | $\mathrm{kg} \mathrm{m}^{2} \mathrm{~s}^{-2}$ |
| Force | Newton | N | $\mathrm{kg} \mathrm{m} \mathrm{s}^{-2}=\mathrm{J} \mathrm{m}^{-1}$ |
| Power | Watt | W | $\mathrm{kg} \mathrm{m}^{2} \mathrm{~s}^{-3}=\mathrm{J} \mathrm{s}^{-1}$ |
| Pressure | Pascal | Pa | $\mathrm{N} \mathrm{m}^{-2}$ |
| Electric charge | Coulomb | C | As |
| Potential difference | Volt | V | $\mathrm{kg} \mathrm{m}^{2} \mathrm{~s}^{-3} \mathrm{~A}^{-1}=\mathrm{J} \mathrm{A}^{-1} \mathrm{~s}^{-1}$ |
| Resistance | ohm | W | $\mathrm{kg} \mathrm{m}^{2} \mathrm{~s}^{-3} \mathrm{~A}^{-2}=\mathrm{V} \mathrm{A}^{-1}$ |
| Frequency | Hertz | Hz | $\mathrm{s}^{-1}$ |

Certain decimal fractions and multiples of SI units have special names (e.g. Angstrom $=$ $10^{-10} \mathrm{~m}$, litre $=10^{-3} \mathrm{~m}^{3}$ ). Though non-SI, use of these units is widespread. The unit 'atmosphere' has special status in thermodynamics and must be retained sometimes as a unit of pressure. One atmosphere is defined as $1.01325 \times 10^{5} \mathrm{~Pa}$ and is most commonly used as a standard pressure, rather than as a unit of pressure. You will also meet the units 'Bar', which equals $10^{5} \mathrm{~Pa}$, and 'torr', which equals $1 / 760$ atmosphere.

It is important to use the accepted symbols. The symbol for gram is g , not gm or gms . It is never correct to add " $s$ " to indicate the plural for a unit. Note also that lower case " $k$ " is used for rate constants (and, in some books, the Boltzmann constant), while upper case " $K$ " means equilibrium constant, or degrees Kelvin - you should make sure these are clearly distinguished in your lab reports (and exam answers!)

## 16 Labelling Graphs and Tables

Confusion often arises when data in a table are shown with a multiplicative power of ten at the head of the table, e.g:

| $\mathrm{T} / \mathrm{K}$ | $10^{6}$ rate $/ \mathrm{s}^{-1}$ |
| :---: | :---: |
| 291 | 4.76 |
| 304 | 6.92 |
| 318 | 9.01 |

Are the values in the 'Rate' column $4.76 \times 10^{-6} \mathrm{~s}^{-1}$, or are they $4.76 \times 10^{6} \mathrm{~s}^{-1}$ ? The rule, stated simply, is "the value in the table is equal to the heading." Thus $4.76=10^{6}$ Rate $/ \mathrm{s}^{-1}$, so Rate $=4.76 \times 10^{-6} \mathrm{~s}^{-1}$. You should adhere to this convention in labelling all graphs and tables. Note the use of the solidus (/) in the heading. It should only be used in this context, not shown as part of the units of a result. i.e., write $40 \mathrm{~km} \mathrm{~s}^{-1}$, not $40 \mathrm{~km} / \mathrm{s}$.

## 17 Checking Your Results

When you have assessed the errors in your experiment, drawn the graphs and completed the calculations, three further tasks must be completed before you can regard your treatment of the results to be finished:

## Are all my results 'reasonable'?

Sometimes, results are quoted which are not just unlikely, but total nonsense (for example, RMMs of $10^{-56} \mathrm{~g} \mathrm{~mol}^{-1}$, or molecular diameters of several metres.) Look at your results to assess whether they are at least of the right order of magnitude. If they are not, your calculations are probably in error. If you have no idea what magnitude they should be, you have not properly prepared for the experiment.

## Are the units of my results appropriate?

## Can I explain any odd-looking results?

If your graph shows excessive scatter of points, there must be a reason. If your results are far away from those expected, there must again be a reason. If you cannot yourself discover the cause of any discrepancy, ask a demonstrator when signing off. But remember: there will not always be someone else to ask, and the primary responsibility for assessing the quality of your results - and explaining what went wrong or right - is your own.

No amount of manipulation of data can rescue a poorly-performed experiment. To get good results from an experiment, you must perform it with care.

## Prepare completely before coming to the laboratory.

Read the entire script for an experiment before you enter the laboratory. Ensure you fully understand what you must do. Try to understand the theory section, even if this covers an area that has not yet been dealt with in lectures.

Plan the experiment in advance.
Do you have to allow instruments to warm up, or water baths to equilibrate? Can you save time by carrying out two parts of the experiment simultaneously? A little advance planning usually saves a lot of time later.

Check that you know what the experiment is designed to accomplish, and how you will accomplish it.

## Check that you understand all safety requirements of the experiment.

If in doubt about an operation, consult a demonstrator or technician.

Think about what you are doing.
Do not slavishly follow instructions; work out why an operation, such as turning a tap on a vacuum line, is required. What will be the result of the operation?

Judge your results critically as the experiment proceeds.
Whenever possible, carry out the calculations required for your report as you do the experiment. Plot your data as you work. Look critically at your results as they accumulate: do they seem reasonable? Can you improve them as you understand more about the experiment? If you do not assess your results while you work, you may be unaware something is seriously wrong until you write your report - by which time it will be too late to repair the damage.

Repeat measurements if they appear to be faulty.
All PTCL experiments can be completed well within the time allotted. You can thus repeat sections of an experiment that seem not to have worked. You can do this on your own initiative, but it may be productive also to discuss with a demonstrator the possible cause of faulty results, and your proposed solution, before repeating a large chunk of experimental work.

