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SIGNIFICANT FIGURES: HOW TO REPORT NUMERICAL RESULTS

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Introduction

Measurements are at the heart of science. As Lord Kelvin once declared, "..... *when you can measure what you are speaking about, and express it in numbers, you know something about it; but when you cannot measure it, when you cannot express it in numbers, your knowledge is of a meagre and unsatisfactory kind.*" Measurements give us quantitative data, from which we can calculate quantitative results. Quantification and statistical analysis of data are among the most important scientific activities, ranging from cutting edge research to routine analysis of samples. Every day, major decisions are made based on chemical analysis of samples, spanning the gamut from agriculture to environment to healthcare.

Every measurement (and every result calculated from measurements) consists of three quantities.

1. A numerical value.
2. A unit (usually, though some measured quantities, such as pH, do not have units).
3. An uncertainty.

Nearly all scientists are perfectly competent at dealing with the first two quantities, but unfortunately tend to forget about the third and its implications. Yet, to ignore or underestimate the uncertainty of a quantitative result, especially one with decision-making implications, is simply bad science.

Consider the analogue scale depicted in Fig. 1, where an instrumental reading is based on the position of a needle on the scale. The reading is clearly a number between 2.5 and 3.0; different workers may legitimately read it as 2.7 or 2.8. While all workers would agree on the first digit (2), there is an uncertainty about the second (7 or 8).

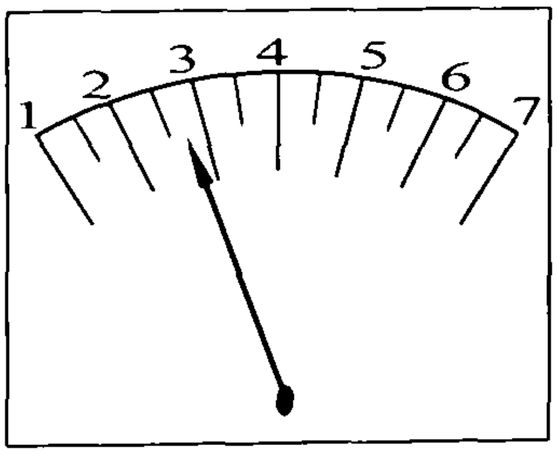

Figure 1. An analogue scale

What about digital instruments? There is a misplaced tendency among many people to place undue faith in a digital display, merely because it is digital. In fact, a digital display does exactly what an observer would do; it estimates the last digit.

Often you can see the last digit changing rapidly while the instrument makes up its mind as to what it should be!

In general, this is true of all measured values. Due to *instrumental uncertainty* (I prefer to avoid the word *error*, which non-scientists equate with *mistake*), all measured values have a number of digits that are *certain* (i.e., all workers would agree on them) plus one which is *uncertain*. This uncertainty carries over into the final result, where it is compounded by other types of uncertainties, e.g.,random and personal ones.

Analytical chemists and scientists doing similar work are (or should be) trained to estimate and report the uncertainty in the final result, together with the result itself. However, I have observed that most research workers, presenting their results at various fora, are extremely careless about the relationship between the accuracy of their measurements and the accuracy of their reported results. A major reason for this is the advent of electronic calculators and, these days, computers running spreadsheets and other programmes for numerical calculations. A proper error analysis is a tedious and time-consuming task. Perhaps this is why people avoid it. However, there is a simple approach which works reasonably well as a "rule of thumb." The approach I am talking about is the concept of *significant figures.*

What Are Significant Figures?

The term *significant figures* refers to the *number of digits* in some value that we are reporting, whether a measurement, or a result calculated from a set of measurements.

521	three significant figures
2.3856	five significant figures
1.6×10^{-4}	two significant figures (expressed in scientific notation)

Let us suppose that we are making a measurement using an analogue instrument. The instrument will contain a scale with calibration marks, and the measurement will typically fall between two of the marks (see Fig. 1). The reading represented by the first of those marks is a definite value with a certain number of digits, all of which are *certain* (*i.e.*, several reasonable individuals making the measurement will all observe the same reading). In addition, we could estimate *one more digit* based on the position of the measurement between the two marks. However, since this is an estimate, different observers may come up with different values for this last digit. Hence, this digit is *uncertain*.

If the calibration marks are so close together that it is impossible to estimate between them, there will be some uncertainty as to which mark represents the best reading. Once again, this results in the last digit being uncertain.

Thus, no matter what kind of measuring device is used, a measurement yields a number, several digits of which may be certain, and the last one uncertain. The total number of certain and uncertain digits is the number of significant figures for that measurement. Obviously one would not report any figures to the right of the uncertain digit, since such figures would be *unknown*.

All of this describes the accuracy with which "raw" data are measured. Of course, such data are seldom reported in scientific papers and presentations. What are reported are the final results, calculated from the raw data. Unfortunately, it is a common practice among far too many scientists, including well-established scientists publishing in international journals, to report these results to absurd numbers of significant figures, without paying the slightest attention to the concept of uncertainty! When challenged, the usual response is to insist that they were following some standard procedure, effectively transferring the responsibility to the originators of that procedure. Others argue that they are merely reporting the results obtained from their computer, or calculator, or even their instrument itself. All scientists have a responsibility to interpret their numerical results and report numbers that make scientific sense, not merely ones that are mathematically correct. Passing the buck amounts to an admission that you do not understand what you are doing. Thus, it is imperative that scientists have some idea of the uncertainty in the results they are reporting, based on the uncertainty in their measurements of raw data, including uncertainties due to statistical fluctuations, and the relationships between such measurements and the calculated results.

Final results cannot be more accurate than the least accurate piece of raw data on which they are based. This is a fundamental principle. It must be interpreted carefully. It does not necessarily mean that the result can only have as many significant figures as the least accurate measurement, though this is usually the case. In certain situations, the actual number of significant figures can be one more or less. The significant figure convention is merely a first approximation, a rule of thumb. It does not completely replace a proper error analysis.

There are some basic rules that govern the relationship between the numbers of significant figures in the data, and those in a calculated result. Before we deal with these rules, we must consider the special role of the zero in significant figures.

When are Zeros Significant?

Rule 1: Zeros between non-zero digits are always significant.

Rule 2: Zeros at the beginning of a number, or which merely serve to locate a decimal point (leading zeros), are never significant.

Rule 3: Zeros at the end of a number *after the decimal point* (trailing zeros) are always significant.

Rule 4: When a number *without* a decimal point ends in zeros, they may or may not be significant, depending on the intent of the reporter. In this situation, if it is important to avoid ambiguity, scientific notation should be used.

The following examples may serve to illustrate these rules.

5008	four significant figures
0.0038	two significant figures (may also be written as 3.8×10^{-3})
21.600	five significant figures
9400	may be two, three, or four significant figures

In the last case, the reporter could be measuring hundreds, tens, or single digits. The situation can be made clear by using scientific notation, based on Rule 3. We could avoid ambiguity by reporting the last number as 9.4×10^3, 9.40×10^3, or 9.400×10^3.

Calculated Results

There are several simple rules which relate the number of significant figures in the final calculated result to the number of such figures in the terms used to calculate it; these terms may be raw data or may themselves be calculated similarly from raw data.

It needs to be clearly understood that, like the entire significant figure convention, the rules given below are "rules of thumb". They are designed to give some indication of *approximately* how many figures a calculated result should have. Properly speaking, every such calculation should be accompanied by at least a crude estimate of the experimental uncertainty. When this is done, it will be much clearer as to how many significant figures the result should be reported. Often this will be one more or less than suggested by the rules given below.

These rules are based on the arithmetical operations used in the calculation.

Rule 1: **Multiplication and Division:** The product or quotient should not have more significant figures than the factor with the least number of significant figures. Provided that no other operation is being used, any number of terms may be multiplied or divided together. It should be remembered that, as the number of terms increases, so does the cumulative uncertainty. *Example: Sodium thiosulphate (2 g, MW 158.11) was dissolved in water and made up to the mark in a 250.00 mL volumetric flask. The molarity of the solution is:*

$$\frac{2\text{ g}}{158.11\text{ g/mol} \times 0.2500\text{ L}} = 0.05\text{ mol/L } (\textit{not } 0.05060\text{ mol/L})$$

The significance of the number of decimals that we record and the uncertainty associated with the measurements and the determination of this uncertainty are also explained.

(If greater accuracy is required, the mass of sodium thiosulphate should be measured, or reported, to the desired number of significant figures. For example, **2.0** *g of sodium thiosulphate would give a concentration of 0.051 mol/L.)*

Rule 2: **Addition and Subtraction:** the absolute value of the uncertainty in a sum or difference is at least as large as the largest uncertainty in any of the terms. In practice this means that the result cannot have more digits to the right of the decimal point than the term with the fewest such digits.

Example: 2.5 kg + 135 g = 2.5 kg + 0.135 kg = 2.6 kg (not 2.635 kg)

A complex formula for calculating the final result may have additions and/or subtractions as well as multiplications and/or divisions. In this situation, the additions and subtractions should be done first, and the resulting terms, to the correct number of significant figures, should be used in the multiplication and division step. It is possible for that number to be quite different from the number of figures in the raw data. For example, consider weighing an unknown sample on an analytical balance, using a watch glass.

weight of watch glass = 19.6893 g
weight of watch glass + sample = 19.7295 g
∴ weight of sample = 0.0402 g

The weight of the sample can be reported to only 3 significant figures, even though the raw data is measured to 6.

Rule 3: **Logarithms:** If a particular number is a logarithm (*e.g.*, pH, pK_a), only the digits *after the decimal point* are significant.

Let us understand the logic behind the last rule. Logarithmic scales of measurement are used when the variable being measured can vary over many orders of magnitude (i.e., powers of 10). The actual values of such variables are usually written in scientific notation, in the format **a** × **10ⁿ**. The significant figures are associated with the term **a**, which is referred to as the *mantissa*. The term **10ⁿ** is the *order of magnitude*, and depends on the units used. The exponent **n**, referred to as the *characteristic*, has *no* significant figures associated with it. It will change if you change the reporting unit, for example from millimetres to micrometres, without, however, changing the accuracy of the original measurement.

Now, if you take the logarithm of this term, the number before the decimal point is derived from the characteristic, **n**. This number (also called the *characteristic*) merely gives the order of magnitude of the measurement, and cannot contribute to significant figures. It is the number after the decimal (the *mantissa*) which is derived from **a**, and is therefore significant.

Consider the following:

$[H^+] = 10^{-7}$: pH = 7 (no significant figures; order of magnitude only)
$[H^+] = 1 \times 10^{-7}$: pH = 7.0 (one significant figure)
$[H^+] = 1.0 \times 10^{-7}$: pH = 7.00 (two significant figures)

Another example of a logarithmic scale is the Richter scale for the strength of earthquakes. An earthquake of magnitude 9.4 is 10 times as powerful as one of magnitude 8.4, both values being reported to one significant figure (which is about how accurately one can estimate the strength of an earthquake).

How many Significant Figures should a Result have?

The answer to this question obviously depends on the nature of the experiment, the instruments used and their accuracy, the spread of random errors, etc. Since a very high proportion of measurements involves analytical chemistry, we can suggest the following guidelines as expectations only.

Gravimetric methods:	4 – 5 figures
Volumetric methods:	3 – 4 figures
Modern instrumental methods:	2 – 3 figures

The latter includes spectrophotometry, electrochemistry, chromatography, etc. These methods enable rapid analysis with high sample turnover and automation, but are not as accurate as the classical methods. The lack of accuracy is often masked by computerized outputs and digital displays. In the analysis of trace components, one should be suspicious of results expressed to more than two figures.

Exact Numbers

The concept of significant figures applies to numbers that have an inherent uncertainty, usually because they are either *measured,* or determined from measured quantities. Some numbers, however, are determined by *counting,* rather than measuring or estimating. In principle, these numbers can be known exactly, i.e., there is no uncertainty. Such exactly known numbers are excluded from the significant figure concept.

Even though they may not be exact, many numbers are known to a much higher degree of accuracy (*i.e.,* many more significant figures) or more exactly than the experiment requires. In addition to counted numbers, they include the following:

- Conversion factors (*e.g.*, multiplying by 2.54 to convert inches into centimetres).
- Certain physical constants that have been determined very accurately (over 12 significant figures in some cases), e.g., speed of light, Avogadro's number.

These numbers are often factors in expressions for various terms, and can be treated as having infinite significant figures for purposes of calculating final results. In other words, they can be ignored from a significant figure.

Statistics and Graphical Methods

Scientists who work with quantitative results, including analytical chemists, are taught that, over and above the instrumental errors such as we have been discussing, there are also random errors in measurement. These are often greater than the expected uncertainties of an instrument's display. In such cases, scientists routinely take several samples, or several aliquots of a gross sample, and make multiple measurements. From these they calculate and present a "best" value (usually a mean, occasionally a median) and some number preceded by a "±" sign (usually a standard deviation, occasionally a confidence interval).

It is important to understand why scientists do this. While others may have various reasons for calculating the standard deviation, scientists almost invariably do so as an expression of the *uncertainty* in their measurement or result. In other words, they give a range of values, within which the "true value" of their measurement or result exists.

If this is the case, I am at a loss to account for reported numbers such as 13.758 ± 2.472. Yet, such numbers abound in both conference presentations and scientific publications. Apparently the scientists who publish such results have no idea why they are calculating a standard deviation, other than that it is something they are supposed to do! In the above case, it is obvious that the *second* digit in the number 13.758 is the uncertain one. If so, the remaining digits are *unknown*, and should not be reported. By the same reasoning, if the number 2.472 represents an uncertainty, to report it to so many significant figures is absurd; how can one be that certain about an uncertainty?

If we adhere strictly to the significant figure convention, the above result should be reported as 14 ± 2. Since the convention is a rule of thumb, some flexibility is permissible. It seldom makes sense to report an uncertainty to more than one figure, but two may be permitted under some circumstances, especially when the first of the two digits is a low one. We can therefore stretch a point and accept 13.8 ± 2.5. However, 13.758 ± 2.472 is absolutely unacceptable. When reporting statistical uncertainties in this way, it is better to use a confidence interval rather than a standard deviation if the number of samples or aliquots is 4 or less.

Many determinations also make use of graphical methods. For example, certain analytical instruments require calibration curves to be drawn, using standard samples. Wherever possible, such curves follow a "$\mathbf{y = mx + b}$" type formula, a classic straight line graph, where **m** is the slope and **b** the intercept. Inevitably, some degree of scatter is present in the raw data used to construct such curves. Nowadays, it is usual to use computers to construct the best line that fits the data, using regression analysis (least squares curve fitting). The computer not only draws a beautiful straight line through the data points, but also calculates the slope and intercept as accurately as you please, together with various other statistical parameters, such as the coefficient of determination, R^2, which is a measure of how good the fit is. Crucially, *the computer can also calculate the standard deviations of m and b*. This is important in estimating the uncertainty in the "graphically" determined results, which can be obtained by substitution into the formula once **m** and **b** are known. Unfortunately, it appears that many workers ignore the uncertainty in **m** and **b**, and report their computed results to quite incredible levels of accuracy.

A good example of this is found in the determination of toxicological parameters such as LD_{50} and LC_{50}, and other similar parameters. LD_{50} and LC_{50} refer to dosages and concentrations, respectively, of some substance, which are lethal to 50% of some test organism, when administered under a given set of conditions. This type of determination is routinely done in a number of sciences – biology, toxicology, pharmacology, natural products chemistry, etc.

Now, let me start by admitting that I am not an expert in this field and have never determined an LD_{50} value. But let us apply common sense to the problem of how accurately such values can be determined. The determination requires a series of dose-response experiments to be carried out, each with a relatively small number of animal subjects, which vary considerably among themselves in the way they respond to the test chemical. While many methods exist to convert this dose-response data into a LD_{50} value, the most accurate methods are graphical. In a typical method, the mortality percentages are converted into "probability units" (probits), and a linear relationship is assumed between the latter and the logarithm of the dose. This linear relationship is obtained by regression analysis, and the dose corresponding to 50% mortality (probit = 5.00) calculated by substitution.

So many variables are present in this determination that it should be obvious that a LD_{50} value is at best an estimate. Objectively, regardless of computed outcomes, it does not seem to me to be possible to determine LD_{50}, LC_{50}, and similar parameters to more than two or at most three significant figures. In fact, standard procedures call for them to be reported with 90% or 95% confidence intervals. If such confidence intervals were calculated, using the results of the regression analysis, I am sure that the opinion I have voiced above would be borne out. However, confidence intervals are seldom reported. Instead, at symposium after symposium, I see LD_{50} and LC_{50} values reported to 4 or even 5 significant figures. Although common sense suggests that such accuracy is impossible (how can one possibly know that exactly 53.86 mg per kg of substance X will kill 50% of the rats exposed to it, as opposed to, say, 53.72?), challenges are met with incomprehension and references to "standard procedures." It appears that too many scientists (and not just Sri Lankan ones!) are only interested in generating a number to put in their paper, and are not overly concerned about exactly what that number *means*.

Rounding-off Errors

The discussion above suggests that too many scientists are reporting their results to too many significant figures, *i.e.*, more accurately than their data justify. While this is true, the opposite problem is still occasionally seen – rounding off data and not making full use of the available accuracy. To be fair, I have observed this problem more with undergraduates than with fully qualified scientists. It usually results from a lack of understanding of the nature of accuracy (*"... 0.0784 is close enough to 0.08, so I will just round it off and use 0.08..."*), coupled to laziness! It can also result from neglecting significant trailing zeroes. For example, many people would re-write 0.60 as 0.6. Mathematically these may be the same number, but scientifically they are quite different, since they imply different levels of uncertainty.

The error associated with expressing your final result to *fewer* significant figures than is justified is obvious, and I will not dwell on it further. This error is carried forward if rounding off takes place at an earlier stage of the calculation; often this leads to a final result that is slightly incorrect. This is known as a rounding-off error. A rounding-off error can occur even if, at an early stage of the calculation, a preliminary result is rounded off to the "correct" number of significant figures. To avoid this, it is a good idea to carry an extra figure or two through the calculation, and only round off to the correct number of significant figures *at the last step*. These extra figures are known as "guard digits."

We can illustrate this with an example. Since I am a chemist, I have chosen an example from elementary chemistry, a typical "A level" problem. Consider the following.

> *A 0.1008 g sample of a mixture of* $FeSO_4$ *and* $Fe_2(SO_4)_3$ *was dissolved in dilute* H_2SO_4*, and titrated with 0.0020 M* $KMnO_4$*. The titration required 15.55 mL of the* $KMnO_4$ *solution. What percent by mass of the mixture was* $FeSO_4$*?*

The stoichiometric relationship between the Fe^{2+} ions in the $FeSO_4$ and the MnO_4^- used as the titrant is shown in the chemical equation below. The data provided allow us to calculate the number of moles of MnO_4^- used, hence the number of moles of Fe^{2+} it reacted with, the mass of the $FeSO_4$ present in the sample, and finally its percentage. We need to know the molar mass (molecular weight) of $FeSO_4$, which is 151.91 g mol^{-1}.

$$5\,Fe^{2+} + MnO_4^- + 8\,H^+ \longrightarrow 5\,Fe^{3+} + Mn^{2+} + 4\,H_2O$$

The first thing to note is that the final answer should be expressed to just two significant figures. This is because the concentration of $KMnO_4$, the least accurately known piece of data, is given to two figures. Such a preliminary estimate of the accuracy of the final answer should become an automatic part of the calculation. However, to express the results of the first step of the calculation (the number of moles of MnO_4^-) to only two figures will, in this case, result in a small error, as shown below.

$$\text{No. of moles of } MnO_4^- = 0.0020\ \text{mol L}^{-1} \times 0.01555\ \text{L} = 3.11 \times 10^{-5}\ \text{mol}$$

If we express the result as 3.1×10^{-5} mol and proceed with the calculation,

$$\text{Mass of } FeSO_4 = 3.1 \times 10^{-5}\ \text{mol} \times 5 \times 151.91\ \text{g mol}^{-1} = 0.024\ \text{g}$$

where 5 is the number of moles of Fe^{2+} per mole of MnO_4^-. The result of the step, 0.02354 g, has been also rounded off to two significant figures and expressed as 0.024 g.

$$\text{Percentage of } FeSO_4 = \frac{0.024}{0.1008} \times 100 = 23.8\% = \mathbf{24\%}\ \text{(after rounding off).}$$

Let us now repeat the calculation while keeping a third digit in the result of each step. This is the *guard digit* mentioned before.

$$\text{Mass of FeSO}_4 = 3.11 \times 10^{-5}\,\text{mol} \times 5 \times 151.91\ \text{g mol}^{-1} = 0.0236\ \text{g}$$

$$\text{Percentage of FeSO}_4 = \frac{0.0236}{0.1008} \times 100 = 23.4\% = \mathbf{23\%}\ \text{(after rounding off).}$$

As you can see, the two ways of doing the calculation give slightly different results. While the difference is small, it is not negligible. Of course, in most cases this round-off error will be insignificant, but it is a good practice to avoid it by using guard digits.

Summary: Mistakes to Avoid

1. Reporting results to too many significant figures, without a correct estimate of the experimental uncertainty. This includes both directly calculated as well as graphically derived results.

2. Reporting standard deviations or confidence intervals, supposedly indications of random error, to more than two significant figures. Usually one figure is enough.

3. Reporting results to too few significant figures, in effect throwing away data. This is rarely seen nowadays except among students.

4. Rounding-off errors, caused by rounding off calculated results prematurely.

Every scientist who works with numbers must make a conscious effort to avoid these elementary mistakes, and to remember that an experimental uncertainty is implicit in every numerical result he or she reports. Eventually, this type of thinking will become second nature, and good scientists will only report numbers that they and their listeners or readers can depend on with confidence.