

Anglo-Chinese School (Independent)

Year 5 (2022) IBDP Chemistry HL



TOPIC 11MEASUREMENT ANDDATA PROCESSING

(IBDP syllabus Topic 11)

- 11.1 Uncertainties and errors in measurement and results (SL and HL)
 - Essential Idea: all measurement has a limit of precision and accuracy, and this must be taken into account when evaluating experimental results
- 11.2 Graphical techniques (SL and HL)
 - Graphs are a visual representation of trends in data

11.1 Uncertainties and Errors in Measurement and Results

Solution Nature of Science:

• Making quantitative measurements with replicates to ensure reliability – precision, accuracy, systematic, and random errors must be interpreted through replication. (3.2, 3.4)

Understandings:

- Qualitative data includes all non-numerical information obtained from observations not from measurement.
- Quantitative data are obtained from measurements, and are always associated with random errors/uncertainties, determined by the apparatus, and by human limitations such as reaction times.
- Propagation of random errors in data processing shows the impact of the uncertainties on the final result.
- Experimental design and procedure usually lead to systematic errors in measurement, which cause a deviation in a particular direction.
- Repeat trials and measurements will reduce random errors but not systematic errors.

Applications and skills:

- Distinction between random errors and systematic errors.
- Record uncertainties in all measurements as a range (+) to an appropriate precision.
- Discussion of ways to reduce uncertainties in an experiment.
- Propagation of uncertainties in processed data, including the use of percentage uncertainties.
 Discussion of systematic errors in all experimental work, their impact on the results and how they can be reduced.
- Estimation of whether a particular source of error is likely to have a major or minor effect on the final result.
- Calculation of percentage error when the experimental result can be compared with a theoretical or accepted result.
- Distinction between accuracy and precision in evaluating results.

Guidance:

- The number of significant figures in a result is based on the figures given in the data. When adding or subtracting, the final answer should be given to the least number of decimal places. When multiplying or dividing the final answer is given to the least number of significant figures.
- Note that the data value must be recorded to the same precision as the random error.
- SI units should be used throughout the programme.

International-mindedness:

• As a result of collaboration between seven international organizations, including IUPAC, the International Standards Organization (ISO) published the *Guide to the Expression of Uncertainty in Measurement* in 1995. This has been widely adopted in most countries and has been translated into several languages.

Theory of knowledge:

• Science has been described as a self-correcting and communal public endeavour. To what extent do these characteristics also apply to the other areas of knowledge?

Aims:

- Aim 6: The distinction and different roles of Class A and Class B glassware could be explored.
- Aim 8: Consider the moral obligations of scientists to communicate the full extent of their data, including experimental uncertainties. The "cold fusion" case of Fleischmann and Pons in the 1990s is an example of when this was not fulfilled.

11.2 Graphical Techniques

Solution Nature of Science:

• The idea of correlation – can be tested in experiments whose results can be displayed graphically. (2.8)

Understandings:

- Graphical techniques are an effective means of communicating the effect of an independent variable on a dependent variable, and can lead to determination of physical quantities.
- Sketched graphs have labelled but unscaled axes, and are used to show qualitative trends, such as variables that are proportional or inversely proportional.
- Drawn graphs have labelled and scaled axes, and are used in quantitative measurements.

Applications and skills:

- Drawing graphs of experimental results including the correct choice of axes and scale.
- Interpretation of graphs in terms of the relationships of dependent and independent variables.
- Production and interpretation of best-fit lines or curves through data points, including an assessment of when it can and cannot be considered as a linear function.
- Calculation of quantities from graphs by measuring slope (gradient) and intercept, including appropriate units.

International-mindedness:

• Charts and graphs, which largely transcend language barriers, can facilitate communication between scientists worldwide.

Aims:

• Aim 7: Graph-plotting software may be used, including the use of spreadsheets and the derivation of best-fit lines and gradients.

Quantitative Chemistry: Errors and uncertainties in chemistry

11.1.1 Why do we learn about Errors and Uncertainties in Chemistry?

The consideration and appreciation of the significance of the concepts of errors and uncertainties helps to develop skills of inquiry and thinking that are not only relevant to the group 4 sciences. The **evaluation of the reliability of the data** upon which **conclusions** can be drawn is at the heart of a wider scientific method, which is explained in section 3 of the "Nature of science" part of the subject guide.

The treatment of errors and uncertainties is also directly relevant to the **internal assessment** criteria of:

- **Exploration** ("The methodology is highly appropriate to address the research question because it takes into consideration all, or nearly all, of the significant factors that may influence the relevance, reliability and sufficiency of the collected data.")
- **Analysis** ("The report shows evidence of full and appropriate consideration of the impact of measurement uncertainty on the analysis.")
- **Evaluation** ("Strengths and weaknesses of the investigation, such as limitations of the data and sources of error, are discussed and provide evidence of a clear understanding of the methodological issues involved in establishing the conclusion.")

Expectations (SL and HL):

Within practical work, students should be able to:

- **design procedures** that allow for relevant data to be collected, in which **systematic errors** are <u>minimized</u> and **random errors** are <u>reduced</u> through the choice of *appropriate techniques and measuring instruments*, and by incorporating *sufficient repeated measurement* where appropriate
- make a quantitative record of **uncertainty range**
- state the results of calculations to the appropriate number of significant figures. The number of significant figures in any answer should reflect the number of significant figures in the given data
- **propagate uncertainties** through a calculation to determine the uncertainties in calculated results and state them as *absolute and/or percentage uncertainties*. Only a simple treatment is required. For functions such as addition and subtraction, absolute uncertainties can be added; for multiplication, division and powers, percentage uncertainties can be added. If one uncertainty is much larger than the others, the *approximate uncertainty* in the calculated result can be taken as due to that quantity alone
- determine from graphs, physical quantities (with units) by measuring and interpreting a slope (gradient) or intercept. When constructing graphs from experimental data, students should make an <u>appropriate choice of axes and scale</u>, and the plotting of points should be clear and accurate. (Millimetre-square graph paper or software is appropriate. Quantitative measurements should not be made from sketch graphs.) The uncertainty requirement can be satisfied by drawing best-fit curves or straight lines through data points on the graph. (Note: Chemistry students are not expected to construct error bars on their graphs.)
- **justify their conclusion** by discussing whether *systematic errors* or *further random errors* were encountered. The **direction** of any systematic errors should be appreciated. The <u>percentage error should be compared with the total estimated random error</u> as derived from the propagation of uncertainties
- comment on the **precision and accuracy** of measurements when evaluating their procedure
- suggest how the effects of random uncertainties may be reduced and systematic errors eliminated. Students should be aware that <u>random, but not systematic, errors are reduced by taking repeated readings</u>.

11.1.2 Decimal Places, Significant Figures and Graph Shapes

(a) Determining the number of decimal places and rounding off

Decimal place refers to the position of a digit to the right of a decimal point. The number of decimal places is determined based on the number of digits to the right of the decimal point. E.g. 3.142 and 0.079 are numbers given to 3 decimal places.

How many decimal places are there for the following numbers?

- 6.63 = <u>2 dp</u>
- 138.0 = <u>1 dp</u>
- 524 = <u>0 dp</u>

Rounding off:

When rounding off a number to a certain number of decimal places, leave the decimal point where it is but look at the number <u>after</u> the one which you want to stop at and round off according to the following rule:

If the number is 5 or above, round the number up. If the number is 4 or below, the number stays the same.

E.g. Rounding off 8.314 to 2 decimal places will leave us with 8.31 and rounding off 3.14159 to 4 decimal places will leave us with a value of 3.1416.

Round off the following numbers to the specified number of decimal places:

- 1.05 = $\frac{1.1}{100}$ (to 1 dp)
- 1.125 = $\underline{1}$ (to whole number)
- 235.010 = <u>235.01</u> (to 2 dp)

(b) Determining the number of significant figures & rounding off

In order to determine the number of significant figures in a measurement the following rules should be applied:

- All non-zero digits are significant. For example, 549 g has three significant figures and 1.892 g has four significant figures.
- Zeros to the left of the first non-zero digit are not significant.
 For example, 0.000034 g has only two significant figures. The value 0.001111 g has four significant figures.
- Zeros between non-zero digits are significant. For example, 4023 g has four significant figures and 50014 g has five significant figures.
- Zeros to the right of the decimal point are significant.
 For example, 2.50 g has three significant figures and 5.500 g has four significant figures.
- If a number ends in zeros that are not to the right of a decimal point, the zeros may or may not be significant.

For example, 1500 g may have two, three or four significant figures.

Numbers like this with trailing zeros are best written in **scientific notation**, where the number is written in the standard exponential form as $N \times 10^n$, where N represents a number with a single non-zero digit to the left of the decimal point and n represents some integer.

The mass above can be expressed in scientific notation in the following forms depending upon the number of significant figures:

- 1.5×10^3 g (2 significant figures)
- 1.50×10^3 g (3 significant figures)
- 1.500×10^3 g (4 significant figures)

In these expressions, all the zeros to the right of the decimal point are significant.

Rounding off:

When rounding off a number to a certain number of significant figures, follow the same rules as when rounding off a number to the nearest decimal place.

If the number is 5 or above, round the number up. If the number is 4 or below, the number stays the same.

E.g. Rounding off 1.125 to 3 significant figures will result in a value of 1.13 and rounding off 0.0054 to 1 significant figure will result in a value of 0.005 or 5×10^{-3} . Round off the following numbers to the specified number of significant figures:

- 0.039 = $\frac{4 \times 10^{-2}}{10^{-2}}$ (to 1 sf)
- 1.145 = $\frac{1.15}{100}$ (to 3 sf)
- 2001 = $\frac{2000 \text{ or } 2.0 \times 10^3}{10^3}$ (to 2 sf)

(c) Conversion between fractions, relative numbers and percentages

The relative comparison of two numbers (e.g. 5 and 10) can be done in the form of a:

1. Fraction:
e.g.
$$\frac{5}{10} = \frac{1}{2}$$

2. Relative number:
e.g. $\frac{5}{10} = 0.5$
3. Percentage:
e.g. $\frac{5}{10} \times 100\% = 50\%$

(d) SI units, Conversion of units and Dimension analysis

SI stands for the International System of Units. The SI base units relevant to the majority of IB chemical measurements and calculations are shown in the following table.

Measurement	Unit	Symbol
Length	metre	m
Mass	kilogram	kg
Time	second	S
Amount	mole	mol
Temperature	Kelvin	K
Electric current	ampere	A

A number of important SI derived units used in IB chemistry are shown in the following table.

Measurement	Unit	Symbol
Frequency	hertz (reciprocal of seconds)	Hz (s ⁻¹)
Pressure	pascal (newton per square metre)	Pa (N m⁻²)
Density	kilogram per cubic metre	kg m⁻³
Heat capacity	joule per kelvin	J K ^{−1}
Specific heat capacity	joule per kilogram per kelvin	J kg ^{−1} K ^{−1}
Heat capacity	joule per kelvin	J K ^{−1}
Entropy	joule per kelvin	J K ^{−1}
Enthalpy change/ gibbs free energy change	joule per mole	J mol ^{−1}
Electrical charge	coulomb	C
Potential difference	volt	V

The sizes of the units are not always the most suitable for certain measurements and decimal multiples are often used. The following table shows the prefixes for common multiples of units.

Multiple	Prefix		
10 ⁻¹²	pico (p)		
10 ⁻⁹	nano (n)		
10 ⁻⁶	micro (μ)		
10 ⁻³	milli (m)		
10 ⁻¹	deci (d)		
10 ³	kilo (k)		
106	mega (M)		

Conversion of units

The conversion of units is very important in Chemistry calculations. Often, you are required to do conversions to convert measurements to their SI units or to ensure units being used in your calculations are consistent.

e.g. 1 m = 100 cm, 1 m³ = 1 x 10^{6} cm³ or 1 x 10^{3} dm³

Dimension analysis

The following rules apply when the equation is homogeneous / dimensionally consistent:

1. Units on both sides of the equation must be consistent: units on LHS = units on RHS

e.g. $n = c \times V$, with n being the amount of substance, c being the concentration and V being the volume.

Units of n = units of $c \times units$ of V

if the units of n and V are mol and dm^3 respectively, units of c = mol / dm^3 = mol dm^{-3}

2. The exponent of a term is dimensionless (no units):

e.g. $e^{-E_a/RT}$ is dimensionless, units of E_a must be equal to units of R x units of T. If R, the molar gas constant has the units of J mol⁻¹ K⁻¹ while T is the absolute temperature in Kelvin, the units of E_a , the activation energy of a reaction must be equals to that of R x T = J mol⁻¹ K⁻¹ x K = J mol⁻¹.

Given that $k = A e^{-E_a/RT}$ where k is the rate constant and A is the Arrhenius constant, and that the units of $k = s^{-1}$, what are the units of A?

Units of LHS = units of RHS, since $e^{-E_a/RT}$ is dimensionless, units of k = units of A = s⁻¹

(e) Types of graphs and manipulation of equations to linearize equations



Common types of mathematical relationships used in sketches and plots:

Linearising of equations:

In the sketching/ plotting of graphs, you are often required to manipulate equations to obtain a linear sketch or plot.

e.g. To sketch / plot a linear graph of p against T,

- 1. Start off from ideal gas equation pV = nRT
- 2. Manipulate ideal gas equation such that only the y-axis variable is on left-hand side of nR_{T}

equation:
$$p = \frac{m}{V}T$$

3. Identify the type of relationship and sketch / plot the graph

If p was sketched / plotted against T, a linear graph would be obtained.



11.1.3 Accuracy, Precision and Types of Errors

(a) Accuracy and precision

Accuracy refers to how close a measured value is to the correct value, whereas **precision** indicates the closeness of agreement between independent test results obtained under stipulated conditions.



Note: **Arithmetic precision** (also commonly known as precision) indicates the number of significant figures/ decimal places a measurement is rounded off to.

For example, a mercury thermometer could measure the normal boiling temperature of water as (100.0 ± 0.5) °C, whereas a data probe may record it as (100.00 ± 0.05) °C. In this case, the data probe is more **precise**.

(b) Types of errors

Systematic errors arise from a problem in the experimental set-up that results in the measured values always deviating from the "true" value consistently in the <u>same</u> direction.

Examples of sources of systematic errors are miscalibration of a measuring device or poor insulation in calorimetry experiments.

- (i) Systematic errors can be minimised or eliminated if the source is known and removed via *modifications to the procedures*.
- (ii) Systematic errors cannot be minimised or eliminated by repeating the experiment and taking the average of the readings.
- (iii) If an experiment has less systematic errors, it is said to have higher accuracy.







Random errors arise from the imprecision of measurements and can lead to readings being above or below the "true" value.

Examples of random errors include fluctuations in temperature or pressure of the environment while the experiment was being carried out.

- (i) Random errors cannot be eliminated even if the source is known.
- (ii) Random errors can be reduced with the use of more precise measuring equipment or their effect can be minimized through repeating measurements and taking the average of the results.
- (iii) If an experiment has less random errors, it is said to have **higher precision**.

Note: In IB, you are often required to evaluate the types of errors which could have affected the experimental results. *Errors or mistakes that occur due to the carelessness or incompetency of the operator should be avoided in your discussion!*

Examples of operator errors include parallax errors, forgetting to rinse the apparatus and misreading of scales.

(c) Uncertainties in raw data

When collecting numerical data, values cannot be determined exactly, regardless of the nature of the scale or the instrument. This is due to two limitations in accuracy of measurement:

- (i) how accurately the instrument is calibrated or the tolerance of the glass apparatus (refer to note on tolerance below), and
- (ii) the skill of the person operating the instrument and/or making the measurement.



The **uncertainty of a measurement** is a range of values which the actual reading lies within.

E.g. If the mass of an object is determined with a digital balance reading to 0.1 g, the actual value lies within a range above and below 0.1g. In other words, if the mass measurement shows on the digital display is 1.0 g, the mass can be anywhere between 0.9 g to 1.1 g and the measurement is recorded as (1.0 ± 0.1) g.

If the same object is measured on a balance which can read up to 0.001 g, the uncertainty is reduced, but it can never be completely eliminated. In this case, the displayed value on the balance is 1.000 g and the actual mass can lie anywhere from 0.999 g to 1.001 g, and the measurement is recorded as (1.000 ± 0.001) g.

In general, the **absolute uncertainty** of a reading **A** is represented by the symbols ΔA (pronounced as "delta A").

There are different conventions for recording **uncertainties in raw data**. As a guide, the Chemistry Department adopts the following conventions.

- The simplest is the **least count**, which simply reflects the *smallest division* of the scale, for example ± 0.001 g on our electronic balance.
- The instrument limit of error, this is usually no greater than the least count and is often a *fraction of the least–count value*.
 E.g. A 50.00 cm³ burette has least count divisions of 0.10 cm³ but is often read to *half of the least-count division* (± 0.05 cm³).
 If the meniscus is at the reading of 23.40 cm³, the burette reading becomes 23.40 cm³ (± 0.05) cm³, following the decimal placing of the uncertainty as it determines the "*arithmetic precision*" of the reading (context here is about how many decimal places).

In summary, the estimated uncertainty takes into account the concepts of **least count** or **instrument limit of error**, as inferred from the tolerance of the instruments, or qualitative considerations related to the estimator's uncertainty / skills such as parallax problems in reading a burette scale or determining the colour change of an indicator or at completion of a reaction, reaction time in starting or stopping a stopwatch, and random fluctuation in a voltmeter or pH probe.

Refer to the list of tolerance / uncertainty values for the common apparatus available in our school laboratories in Section 11.1.7.

Note: The tolerance (uncertainty values of apparatus) are determined by the manufacturers. Apparatus are classified according to *Class A* or *Class B*. *Class A apparatus have very low tolerances compared to Class B apparatus*. Class A apparatus has glass that is a lot thinner to allow for quick expansion or contraction when temperature changes and are costlier.

As a guide, the tolerances of Class B apparatus are usually twice that of their equivalent Class A apparatus, and they are all temperature specific (must be used at the temperature marked on the apparatus because volume changes with temperature).

The experimental reading **A** together with its absolute uncertainty is expressed in the form of $(A \pm \Delta A)$. For example, the mass of an object is (0.500 ± 0.001) g.

In general, express

- the absolute uncertainty of (ΔA) to one significant figure for measurements
- the measured value (A) to the same decimal place as the uncertainty
- for propagated absolute uncertainties both with the same units
- e.g. (34.10 ± 0.05) cm³

11.1.4 Fractional and Percentage Uncertainties

Uncertainties can also be represented in the form of:

- Fractional uncertainty = $\frac{\Delta A}{A}$
- Percentage uncertainty = Fractional uncertainty x 100 % = $\frac{\Delta A}{A}$ x 100 %

The fractional / percentage uncertainty gives an indication of the significance of the error and the suitability of the instrument used in the measurement.

Note: A small reading (A) can give rise to a large fractional / percentage uncertainty.

Conversions between absolute and percentage uncertainties

Note: The usage of absolute and percentage uncertainties are more common in chemistry literature.

Example 1.

The concentration of a solution is determined to be 0.0050 mol dm⁻³ (\pm 2%). Absolute uncertainty = \pm (2% x 0.0050) = \pm 0.0001 mol dm⁻³. So the concentration can be expressed as (0.0050 \pm 0.0001) mol dm⁻³.

Example 2.

The density of a gas is determined to be 0.0050 g cm⁻³ (\pm 1.5%) Absolute uncertainty = 1.5% x 0.0050 = 0.000075 g cm⁻³. So the concentration can be expressed as (0.0050 \pm 0.0001) g cm⁻³.

Note:

It is incorrect to express it as (0.0050 ± 0.000075) g cm⁻³ due to the inconsistency in the number of decimal places between the calculated concentration (4 dp) and its absolute uncertainty (6 dp). As the decimal place of the concentration cannot increase beyond 4 (or significant places increase beyond 1), it is preferred to increase the magnitude of the uncertainty to 0.0001 g cm⁻³ to so that true value still falls within the new range from 0.0049 g cm⁻³ to 0.0051 g cm⁻³.

11.1.5 Propagating Errors

In the processing of data, the random error in the final calculated result can be propagated based on the random errors (uncertainties) in the raw data.

There is a range of protocols for **propagating errors**:

(i) When adding or subtracting quantities, the absolute uncertainties of the quantities are added.

E.g. If the initial and final burette readings in a titration each have an uncertainty of $\pm 0.05 \text{ cm}^3$ then the propagated **absolute uncertainty** for the total volume is: $(\pm 0.05 \text{ cm}^3) + (\pm 0.05 \text{ cm}^3) = (\pm 0.10 \text{ cm}^3).$

(ii) When multiplying or dividing quantities, the percentage uncertainties / fractional uncertainties of the quantities are added.

L.y.	
Concentration of NaOH (ag)	Percentage uncertainty of conc of NaOH
(4,00,0,05) as a laber ³	
$= (1.00 \pm 0.05) \text{ mol am}^{\circ}$	
	$= \left[\frac{1.00}{1.00}\right] \times 100\% = 5\%$
volume of NaOH (ag)	Percentage uncertainty of vol of NaOH
$-(10.0 \pm 0.1)$ cm ³	01
$=(10.0 \pm 0.1)$ cm	$= [] \times 100 \% = 1 \%$
	10.01

Therefore, calculated no. of moles of NaOH in solution

Note: 3 sf for final answer (lowest no. of sf)

 $= 1.00 \times \left[\frac{10.00}{1000}\right] = 0.0100 \text{ moles } (\pm 6\%) \text{ or } (0.0100 \pm 0.0006) \text{ mol.}$

Note that it is one sf for the both the percentage and absolute uncertainties but zero and four decimal places for them respectively.

(iii) When multiplying or dividing by a constant, k, the absolute uncertainty changes by a factor of k and the percentage uncertainties of the quantities remain constant.

E.g. (20.10 \pm 0.10) cm³ x 3 = (60.30 \pm 0.30) cm³ while percentage uncertainty remains constant at 0.50 % after the multiplication.

A common protocol is that the final total percentage uncertainty should be cited to:
no more than one significant figure if it is greater than or equal to 2%

no more than one significant figure if it is less than or equal
 no more than two significant figures if it is less than 2%

no more than two significant figures if it is less than 2%.

A common protocol is that the final total absolute uncertainty should be cited to:

no more than one significant figure.

How many decimal places / significant figures should the final answer have?

- When adding or subtracting quantities, *final answer* follows the lowest number of decimal places of the raw data used in its computation.
- When multiplying or dividing quantities, *final answer* follows the **lowest significant figure** of the raw data used in its computation.
- Ultimately, final answer should have the same number of decimal places as absolute uncertainty.

How many decimal places/ significant figures should the intermmediate answer have?

• Intermmediate answer follows the lowest number of significant figures or decimal places according to rules stated above for the final answer, with reference to the raw data used in its computation, to ensure accuracy when it is used in subsequent calculations.

Example 1

 (20.00 ± 0.05) g of sugar is dissolved in (50.00 ± 0.10) cm³ of distilled water. Find its concentration in g cm⁻³.

Absolute value calculation		Percentage uncertainty determination				
Mass of sugar	= (20.00 ± 0.05) g [2 dp and 4 sf]		Percentage uncertainty in mass reading = $\frac{0.05}{20.00} \times 100 \% = 0.3 \%$ (1 sf, lowest sf, rounded up)			
Volume of solution	= (50.00 ± 0.10) cm [2 dp and 4 sf]	3	Percentage uncertaint = $\frac{0.10}{\frac{50.00}{(2 \text{ sf, be})}}$	Percentage uncertainty in volume reading = $\frac{0.10}{50.00} \times 100 \% = 0.20 \%$ (2 sf, lowest sf, rounded up)		
Concentration of sugar solution $= \frac{20.00}{50.00}$ $= 0.4000 \text{ g cm}^{-3}$ (4 sf, lowest sf)			Percentage uncertainty of concentration = $0.3 \% + 0.20 \%$ = 0.5% (1 dp, lowest dp, rounded up)			
Absolute uncertainty of concentration		= 0 = 0	0.4000 x 0.5 %Note:0.002 g cm ⁻³ 1 sf for calculated absolute uncertainty			
So, concentration of s	ugar	= ((0.400 \pm 0.002) g cm ⁻³ 3 dp for both final answer and ab	solute uncertainty)		

Example 2a

 (2.355 ± 0.002) g of a weak organic monoprotic acid was dissolved in (250.00 ± 0.30) cm³ distilled water using a volumetric flask. (20.00 ± 0.06) cm³ of the acid solution was then titrated with (0.100 ± 0.005) mol dm⁻³ sodium hydroxide standard solution and the results are given in the following table. Determine the molar mass of the organic monoprotic acid.

Titration number	1	2	3
Final volume of aqueous NaOH / cm ³ (± 0.05)	25.70	25.40	25.45
Initial volume of aqueous NaOH / cm ³ (± 0.05)	0.00	0.00	0.00
Volume of aqueous NaOH required / cm ³ (± 0.10)	25.70	25.40	25.45
Titration used		\checkmark	\checkmark

Note: precise readings (consistent readings within the difference of ± 0.10 cm³) are used to calculate the mean instead of using all readings.

Absolute value calculation	Percentage uncertainty determination		
Mass of weak organic acid = (2.355 ± 0.002) g	% uncertainty of mass of weak organic acid $= \frac{0.002}{2.355} \times 100 \%$ $= 0.09 \%$ (1 sf, lowest sf, rounded up)		
Concentration of NaOH = (0.100 ± 0.005) mol dm ⁻³	% uncertainty of concentration of NaOH = $\frac{0.005}{0.100} \times 100$ % = 5 % (1 sf, lowest sf, rounded up)		
Average volume of NaOH used = $\frac{25.40 + 25.45}{2}$	% uncertainty for volume of aqueous NaOH = $\frac{0.10}{25.43} \times 100 \%$		
$= (25.43 \pm 0.10) \text{ cm}^3$	= 0.40 % (2 sf, lowest sf, rounded up)		
Volume of organic acid used (via pipette) = (20.00 ± 0.06) cm ³	% uncertainty for volume of organic monoprotic acid in pipette $= \frac{0.06}{20.00} \times 100 \%$ $= 0.3 \%$ (1 sf, lowest sf, rounded up)		
Concentration of acid solution $= \frac{25.43}{20.00} \times 0.100$ $= 0.127 \text{ mol dm}^{-3}$ (3 sf, lowest sf, rounded off)	% uncertainty of concentration of acid = % uncertainty of concentration of NaOH + % uncertainty of volume of NaOH + % uncertainty of of volume of acid = 5 % + 0.40 % + 0.3 % = 6 % (0 dp, lowest dp, rounded up)		

Absolute value calculation	Percentage uncertainty determination
Volume of acid solution prepared using 250 cm ³ volumetric flask = (250.00 ± 0.30) cm ³	% uncertainty of volume of acid solution $= \frac{0.30}{250.00} \times 100 \%$ $= 0.12 \%$ (2 sf, lowest sf, rounded up)
No. of moles of acid used in preparing $250 \text{ cm}^3 \text{ stock solution}$ $= 0.127 \times \frac{250.00}{1000.00}$ $= 0.0318 \text{ mol}_{(3 \text{ sf, lowest sf, rounded off)}}$	% uncertainty of no. of moles of acid in 250 cm ³ stock solution = $0.12 \% + 6 \%$ = 6.12% = 7% (0 dp, lowest dp, rounded up)
Mass of 0.0318 mol of acid = 2.355 g	
Therefore molar mass of acid $= \frac{2.355}{0.0318}$ $= 74.1 \text{ g mol}^{-1}$ (3 sf, lowest sf, rounded off)	% uncertainty of molar mass = $0.09 \% + 7 \%$ = 7.09% = 8% (0 dp, lowest dp, rounded up) Absolute uncertainty of molar mass = $74.1 \times 8 \%$ = 5.928 = 6 g mol^{-1} (1 sf for absolute uncertainty, rounded up)

So, molar mass of acid = (74 ± 6) g mol⁻¹ (0 dp for both final answer and absolute uncertainty)

Note:

- The lowest number of significant figures comes from the concentration of NaOH, which is
 3. Hence, the final answer, molar mass = 74.1 g mol⁻¹, will contain no more or less than
 3 significant figures.
- The final answer should have the same number of decimal places as absolute uncertainty. In this case, as the absolute uncertainty has 0 decimal places, the final answer should also have 0 decimal places.

Example 2b

 (2.355 ± 0.002) g of a weak organic monoprotic acid was dissolved in (250.00 ± 0.30) cm³ distilled water in a volumetric flask. (20.0 ± 0.5) cm³ of the acid solution was then titrated with (0.100 ± 0.005) mol dm⁻³ sodium hydroxide standard solution. The results obtained are given in the following table. Determine the molar mass of the organic monoprotic acid.

Titration number	1	2	3
Final volume of aqueous NaOH / cm ³ (± 0.05)	25.70	25.40	25.45
Initial volume of aqueous NaOH / cm ³ (± 0.05)	0.00	0.00	0.00
Volume of aqueous NaOH required / cm ³ (± 0.10)	25.70	25.40	25.45
Titration used		\checkmark	\checkmark

Note: precise readings (consistent readings within the difference of ± 0.10 cm³) are used to calculate the mean instead of using all readings.

Absolute value calculation	Percentage uncertainty determination		
Mass of weak organic acid = (2.355 ± 0.002) g	% uncertainty of mass of weak organic acid $= \frac{0.002}{2.355} \times 100 \%$ $= 0.09 \%$ (1 sf, lowest sf, rounded up)		
Concentration of NaOH = (0.100 ± 0.005) mol dm ⁻³	% uncertainty of concentration of NaOH = $\frac{0.005}{0.100} \times 100 \%$ = 5 % (1 sf, lowest sf, rounded up)		
Average volume of NaOH used = $\frac{25.40 + 25.45}{2}$ = (25.43 ± 0.10) cm ³	% uncertainty for volume of aqueous NaOH = $\frac{0.10}{25.43} \times 100 \%$ = 0.40 % (2 sf, lowest sf, rounded up)		
Volume of organic acid used (via measuring cylinder) = $(20.0 \pm 0.5) \text{ cm}^3$	% uncertainty for volume of organic monoprotic acid in measuring cylinder $= \frac{0.5}{20.0} \times 100 \%$ $= 3 \%$ (1 sf, lowest sf, rounded up)		
Concentration of acid solution $= \frac{25.43}{20.0} \times 0.100$ $= 0.127 \text{ mol dm}^{-3}$ (3 sf, lowest sf, rounded off)	% uncertainty of concentration of acid = % uncertainty of concentration of NaOH + % uncertainty of volume of NaOH + % uncertainty of volume of acid = 5 % + 0.40 % + 3 % = 8.40 % = 9 % (0 dp, lowest dp, rounded up)		

Absolute value calculation	Percentage uncertainty determination			
Volume of acid solution prepared using 250 cm ³ volumetric flask = (250.00 ± 0.30) cm ³	% uncertainty of volume of acid solution $= \frac{0.30}{250.00} \times 100 \%$ $= 0.12 \%$ (2 sf, lowest sf, rounded up)			
No. of moles of acid used in preparing 250 cm ³ stock solution $= 0.127 \times \frac{250.00}{1000.00}$ $= 0.0318 \text{ mol}_{(3 \text{ sf, lowest sf, rounded off)}}$	% uncertainty of no. of moles of acid in 250 cm ³ stock solution = $0.12 \% + 9 \%$ = 9.12% = 10% (0 dp, lowest dp, rounded up)			
Mass of 0.0318 mol of acid= 2.355 g				
Therefore molar mass of acid $= \frac{2.355}{0.0318}$ $= 74.1 \text{ g mol}^{-1}$ (3 sf, lowest sf, rounded off)	% uncertainty of molar mass = $0.09 \% + 10 \%$ = 10.09% = 11% (0 dp, lowest dp, rounded up) Absolute uncertainty of molar mass = $74.1 \times 11 \%$ = 8.151 g mol^{-1} = 9 g mol^{-1} (1 sf for absolute uncertainty, rounded up)			

So, molar mass of acid = (74 ± 9) g mol⁻¹ (0 dp for both final answer and absolute uncertainty)

Note:

The usage of different apparatus resulted in different degree of random errors in examples • 2a and 2b. The usage of a less precise instrument (measuring cylinder) in example 2b led to significantly higher uncertainty in the final calculated molar mass of acid. In research, it is important to take the uncertainties of the apparatus into consideration.

11.1.6 Repeated Measurements

Repeated measurements can be averaged to represent a quantity. In research, it is important to replicate the procedures till precise data is obtained. **In averaging, only the precise values are considered and outliers are omitted** and in the process, random uncertainties (errors) are reduced.

The final answer may be given using the propagated error of the component values that make up the average. If the rule of adding up the absolute uncertainty applies, then the overall uncertainty will swell in accordance to the number of measurements used which does not make any sense and contradicts to the concept that it improves the measurement by reducing the random uncertainty. The two examples below illustrate this further.

Example 1

In a volumetric analysis, the following volumes are obtained for the titre (in cm³):

Titration number	1	2	3	4	5
Final volume of aqueous NaOH	21.05	21.10	21.00	20.95	21.35
/ cm ³ (± 0.05)					
Initial volume of aqueous NaOH	0.00	0.00	0.00	0.00	0.00
$/ \text{ cm}^3 (\pm 0.05)$					
Volume of aqueous NaOH required	21.05	21.10	21.00	20.95	21.35
$/ \text{ cm}^3 (\pm 0.10)$					
Titration used	\checkmark		\checkmark	\checkmark	

Considering only the precise values, only 21.05, 21.00 and 20.95 will be used for averaging the calculated average is 21.00.

The uncertainty of the titre used is $0.05 + 0.05 = \pm 0.10$ cm³, considering that the final reading and initial reading each has an uncertainty of ± 0.05 cm³.

Absolute value calculation	Percentage uncertainty determination
Average titre volume	Absolute uncertainty of mass of weak organic acid
21.05 + 21.00 + 20.95	0.10 + 0.10 + 0.10
=3	$=\frac{3}{3}$
= 21.00 cm ³ (2 dp, lowest dp)	= 0.10 cm ³ (summation of absolute uncertainties in an addition, followed by division of 3)

The average volume of titre used is 21.00 cm^3 and the absolute uncertainty remains constant at $\pm 0.10 \text{ cm}^3$.

Example 2

In another volumetric analysis, a student decided to perform 30 sets of procedures and obtained the following data:

Volume of titre (cm ³)	20.85	20.90	20.95	21.00	21.05	21.10	21.15	21.20
Frequency	2	2	8	7	7	2	1	1

The student decides to average using all the values and calculated it to be 21.00 cm^3 . He then **erroneously** added all the uncertainties which works out to be $\pm 3.00 \text{ cm}^3$ and reported his calculated volume as $(21.00 \pm 3.00) \text{ cm}^3$, and that raised his uncertainty to almost 15%. So if the student decides to collect 300 sets of data, his percentage uncertainty will swell to 150%, more than the average volume of titre itself.

Note:

A more rigorous method for treating repeated measurements is to calculate standard deviations and standard errors (the standard deviation divided by the square root of the number of trials). These statistical techniques are more appropriate to large-scale studies with many calculated results to average. This is not common in IB chemistry and is therefore not a requirement in chemistry internal assessment.

11.1.7 Making Sense of Error Data in IA

What you can infer if your experimental data differs greatly from the literature data

Investigations requiring you to determine an already known and accepted value of a physical quantity such as the standard enthalpy of neutralisation, the melting point of a substance or the value of the ideal gas constant is common. In such investigations, it is *mandatory for the random error / propagated uncertainty and the* **experimental error / percentage difference** to be calculated.

Evperimental error / percentage difference -	Experimental value – Literature value	
Experimental error / percentage difference =	Literature value	X 100 %

Quite often, your experimentally measured quantity differs greatly from the literature value and thus, your **experimental error (percentage difference)** is high, and there are two possible explanations to the discrepancy between your experimental value and the literature value.

1. The presence of systematic errors

When the experimental error (percentage difference) is more than the calculated error (propagated percentage uncertainty), systematic error is definitely present.

For example, a student measured the value of the ideal gas constant, R, to be 8.11 kPa dm³ mol⁻¹ K⁻¹ with an uncertainty of 2%, and the accepted value is 8.314 kPa dm³ mol⁻¹ K⁻¹.

Percentage difference = $\left|\frac{8.11 - 8.314}{8.314}\right| \times 100 \% = 2.45 \%$ (3 sf, lowest sf) The error (a measure of accuracy, not precision) is 2.45% of the accepted value. Random

The error (a measure of accuracy, not precision) is 2.45% of the accepted value. Random errors alone cannot explain the difference (because the difference is more than the calculated uncertainty) and some systematic error(s) is definitely present.

2. There are uncertainties that are not considered

The difference can also be caused by an uncertainty that is underestimated and there must be more uncertainty and / or errors than have been acknowledged. Also, there is a likelihood that the uncertainty reported could be lower than what it should be.

In addition, students may also comment on errors in the **assumptions** of the theory being tested, and errors in the method and equipment being used. Two typical examples of student work are given in **Figures 1 and 2**.



Intermolecular bonds are being broken and formed, which will affect the energy change. There is a definite correlation between the melting point and the freezing point of a substance. If good data is collected, the melting point should be the same as the freezing point. A substance should melt, go from solid to liquid, at the same temperature that it freezes, goes from liquid to solid. Our experiment proved this is true because, while freezing, the freezing point was found to be 55°C, and when melting, the melting point was also found to be 55°C (see graph).

Note: The student above states a conclusion that has some validity. However, no comparison is made with the literature value and there is no evaluation of the procedure and results. For IA, this would contribute to low marks in the analysis and evaluation criteria.



Melting point = freezing point = $55.0 \pm 0.5^{\circ}C$

Percentage uncertainty = $\frac{0.5}{55.0}$ × 100 = 0.9 % (1 sf, lowest sf)

Literature value of melting point of para–dichlorobenzene = 53.1° C (Handbook of Chamistry and Physics, Haynes, WM, (2012) CPC pross)

(Handbook of Chemistry and Physics, Haynes, W.M. (2012) CRC press).

Percentage difference = $\left|\frac{55.0 - 53.1}{53.1}\right| \times 100 \% = 3.58 \% (3 \text{ sf, lowest sf})$

The fact that % difference > % uncertainty means random errors alone cannot explain the difference and some systematic error(s) must be present.

Melting point (or freezing point) is the temperature at which the solid and the liquid are in equilibrium with each other: (s) \Rightarrow (l). This is the temperature at which there is no change in kinetic energy (no change in temperature), but a change in potential energy. The value suggests a small degree of systematic error in comparison with the literature value as random errors alone are unable to explain the percentage difference.

Evaluation of procedure and modifications:

- Duplicate readings were not taken. Other groups of students had % uncertainty > % difference, that is, in their case random errors could explain the % difference, so repeating the investigation is important.
- The thermometer should have been calibrated. In order to eliminate any systematic errors due to the use of a particular thermometer, calibration against the boiling point of water (at 1 atmosphere) or better still against a solid of known melting point (close to the melting point of the sample) should be done.
- The sample in the test tube was not as large as in other groups. Thus the temperature rises/falls were much faster than for other groups. A greater quantity of solid, plus use of a more accurate thermometer (not 0.5°C divisions, but the longer one used by some groups) would have provided more accurate results.
- For IA, this could contribute to the attainment of the highest levels in the analysis and evaluation criteria.

Additional notes:

(a) Computation with special functions and uncertainties

In some topics, special functions such as *log*, *ln*, *log*⁻¹, *ln*⁻¹, etc. are used in chemistry calculations. You will encounter some of them in Kinetics this year and Ionic Equilibria next year. In determining the total uncertainty of a calculation that involves special function like the log function (which will be used to illustrate here), one has to determine the upper and lower limit of the reading and the log function of these limits. Then average both logged limits to determine the logged reading, and determine the uncertainty range by finding the difference between the upper and lower limits of the logged readings and halving it.

Example

The concentration of hydrochloric acid is (1.50 ± 0.05) mol dm⁻³. Assuming complete dissociation of the HCl molecules into ions in water, find the *pH* of the acid.

Since hydrochloric acid is monoprotic and completely dissociates in water,

 $[HCl] = [H^+]$ (or $[H_3O^+]$) = (1.50 ± 0.05) mol dm⁻³

Lower limit:

 $[H^+] = 1.45 \text{ mol } dm^{-3}$ $pH = -lg [H^+] = -lg (1.45) = -0.161$

Upper limit:

 $[H^+] = 1.55 \text{ mol } dm^{-3}$ $pH = -lg [H^+] = -lg (1.55) = -0.190$

 $pH = -\lg [H^+] = -\lg (1.50) = -0.176$

Uncertainty between upper limit and pH = -0.161 - (-0.176) = 0.015Uncertainty between lower limit and pH = -0.176 - (-0.190) = 0.014

So, 0.015 is the larger uncertainty.

Therefore, *pH* of hydrochloric acid = -0.176 ± 0.015

(b) Uncertainties of common apparatus in IB Chemistry Laboratories

Capacity / cm ³	Measuring cylinder / cm ³	Volumetric flask / cm ³	Burette* / cm ³	Graduated pipette / cm ³	Bulb pipette / cm ³
1				±0.01 (B)	
2				±0.02 (B)	
5				±0.05 (B)	
10	±1.0	±0.02 (A)		±0.04 (A)	±0.02 (A)
		±0.05 (B)		±0.1 (B)	
20				±0.06 (B)	±0.03 (A)
					±0.06 (B)
25		±0.08 (B)			
50	±0.5	±0.12 (B)	±0.05* (B)		±0.10 (A)
100	±0.8	±0.08 (A)			±0.15 (A)
		±0.20 (B)			
250		±0.12 (A)			
		±0.3 (B)			
500		±0.25 (A)			
		±0.5 (B)			
1000		±0.8 (B)			

(Class of apparatus, if any, is denoted in parenthesis)

* Need to multiply by 2 for initial and final readings.

Measurement uncertainty of instruments in IB Chemistry Laboratories

Instrument	Brand /Model (if any)	Uncertainty	Operating Temperature	Website for reference
Electronic balance*	Precisa XT 220A	±0.001 g*	5 to 40 ^o C	http://www.precisa.com /download/en_320XT_ Handbook.pdf
Thermometers • 0.2 ^o C division • 0.5 ^o C division	-	±0.2 °C ±0.5 °C	0 to 100 ^o C	
Stopwatch	Sport Timer/ TM-104	±0.5 s	Room temperature	
Data Logger • pH probe • temperature probe	Vernier • PH-BTA • WRT-BTA	±0.02 pH ±0.2 °C	5 to 80 ^o C -40 to <40 ^o C	pH probe: http://www.vernier.com /files/manuals/ph- bta.pdf <u>Temperature probe:</u> http://www.vernier.com /products/sensors/temp erature-sensors/tpl- bta.pdf
UV-Vis Spectrometer (190 to 1100 nm)	Genesys 10S	±0.005 A (<1 A) ±0.5% of reading (1-2 A)	Room temperature	http://www.thermo.com /eThermo/CMA/PDFs/ Product/productPDF_5 3056.pdf

Shimadzu UV1800	±0.004 A (<1 A)	
	±0.006 (1-2 A)	

* Need to multiply by 2 for initial and final readings.

Theory of knowledge

"Science has been described as self-correcting and communal public endeavor. To what extent do these characteristics also apply to the other areas of knowledge?"

Note: The five areas of knowledge in TOK are natural sciences, human sciences, ethics, the arts and mathematics.

Question for consideration:

Why has the value of Avogadro's constant changed over time?

International-mindedness

"As a result of collaboration between seven international organizations, including IUPAC, the International Standards Organization (ISO) published the Guide to the Expression of Uncertainty in Measurement in 1995. This has been widely adopted in most countries and has been translated into several languages."

Question for consideration:

Consider the pros and cons of adopting an international standard. Explain whether it will be advantageous for Singapore to adopt an international standard.

11.2 Graphical Techniques

One simple approach is to determine if there is any correlation between different sets of data, and if one exists, to determine if there is any cause and effect relationship. Such findings assist to simplify the scientific world into simple models and these have boundless applications in making predictions and solving problems. Hence, *the idea of correlation* will always be the first analytical approach that comes to the minds of researchers and *can be tested in experiments whose results can be displayed graphically* through either manual plotting on a graph paper or through the use of many different graph plotting software.

11.2.1 Sketch Graphs to Represent Dependences and Interpret Graph Behaviour

Graph plotting is an integral part of both data presentation and analysis in most scientific research. It allows the researcher to see the type of relationship between two variables, or that there is any relationship between them. Figures A to E show some of the possible relationships that you may encounter in your IBDP Chemistry course.



Figure A

Significant positive correlation between X and Y. Y = mX, where *m* is refers to the gradient which is positive.





Insignificant correlation between X and Y. There is no relationship between X and Y.





Figure B

Significant negative correlation between X and Y. Y = mX, where m is refers to the gradient which is negative.





Significant positive correlation between X^n and Y. Equation of the line can be generalized as $Y = mX^n$, where *m* is refers to the gradient which is positive, and n any real number. In such cases,

 $\ln Y = n \ln X + \ln m$ will be a straight line.



X is dependent on Y. However, it is not easy to find an equation for such a line.

11.2.2 Construct Graphs from Experimental Data

Graph construction procedure

- 1. Select a full piece of graph paper of at least A4 size. Plan to use the entire graph paper for each plot.
- 2. Draw the axes and use suitable scales such as multiples of 1, 2, 5, 10, etc. such that the graph can encompass the point with the largest and smallest co-ordinates. Never use scales that are difficult to read, such as multiples of 3, 4, 6, 7, etc. If the numbers are too big or too small, convert them into the standard form as shown in Figure 3 below.
- 3. Plot the points carefully on the graph paper using crosses (or any suitable symbols) that are large enough to be seen clearly.
- 4. Label the axes and include the units.
- 5. Label the graph and refer to the graph when you write your report.



Figure on use of standard form in horizontal axis in graph plotting, extracted from 2011 May HL Chemistry Paper 2 TZ1

11.2.3 Error Bars

In some instances, such as in writing Extended Essays, you may wish to show the error bars for all the points in your graph. This is not a requirement in IBDP Chemistry and is entirely up to you. If error bars are used, it should encompass both the horizontal and vertical uncertainties. An example of a graph with error bar is shown below in **Example 1** where the rise in temperature is extrapolated. One common misconception is that the line must pass through all the error bars. In any experiment, anomalous results may occur and such points should still be omitted. The line should only pass through the error bars if you are considering those points as "accurate points".

Example 1



11.2.4 Draw Best-Fit Lines through Data Points on a Graph

The **best-fit-line** can easily be determined using any graph plotting software. In statistics, "linear regression" is used to analyse the relationship between two variables, X and Y. In some situations, the line must pass through the origin as that is a theoretical point. In other cases, the vertical axis intercept yields a significant piece of information.

If you are manually plotting the graph on your own, you may estimate the best-fit-line by adjusting the ruler to a position where all the points are very close to the line. You may also encounter anomalous points and must know how to deal with them. This anomalous point should either be ignored in drawing the best-fit-line, or the experiment can be repeated to obtain a new set of data.

11.2.5 Determine the Values of Physical Quantities from Graphs

From a graph plot, a researcher not only can see the relationship, but also derive some of the physical quantities. The most common quantities are derived from reading the co-ordinates of a point on the line, the gradient of the straight line or the intercept. The following are some examples.



Source: Hutchinson, J. S. The Ideal Gas Law. Silverman, J. Ed., 16 Jan 2005; Connexions. http://cnx.org/content/m12598/latest_(accessed Jan 25,

At constant pressure, the gradient of the above line in **Example 1** yields *nR*, where *n* is the number of moles of the gas and *R* is the ideal gas constant.

Example 1

Example 2



From the Beer–Lambert plot, one can determine the concentration of copper(II) ions by measuring its absorbance using UV–Visible Spectrometry. From the graph, the absorbance of 0.65 of a solution of copper(II) ions corresponds to a concentration of 0.0035 mol dm⁻³. If we consider the uncertainty of the absorbance as \pm 0.05 and extrapolate the upper and lower limits to the line, we should be able to obtain the uncertainty of the concentration, which is \pm 0.0003 mol dm⁻³.

Note: Each of our UV–Visible Spectrometers has an absorbance tolerance of \pm 0.005 and not \pm 0.05 as in the above example.

Example 3



In the *pH* plot above that involves a titration between a strong acid and a weak base, three valuable pieces of information that can be obtained from the *pH* axis; the *pH* of the acid before titration (point A), the *pH* of the base (point B) (which allows you to derive its concentration if you know its *pK*_b value) and the *pH* at equivalence point (point C).

11.2.6 Software for Graph Plotting

There are many software available for graph plotting with error bars and best-fit-line:

- 1. Microsoft Excel available as a bundle with Word and PowerPoint. You may use the software in the Shaw Library's computers.
- 2. SPSS PASW Statistics Student Version 18 rather expensive and license lasts 13 months.
- 3. Graph ver 4.3 developed by Ivan Johansen in 2009 this is a freeware and can be downloaded from http://www.padowan.dk/graph/

Theory of knowledge

"Graphs are a visual representation of data, and so use sense perception as a way of knowing. To what extent does their interpretation also rely on the other ways of knowing, such as language and reason?"

International-Mindedness

"Charts and graphs, which largely transcend language barriers, can facilitate communication between scientists worldwide."

Question for consideration:

We see charts and graphs so commonly used in the mass media. How effective are such visual tools in communicating the same ideas and transcending across different nationalities with vastly different languages, cultures, traditions, values and beliefs?

Clue: Consider the minimal language or words used such as labeling of axes, title of graphs or charts, versus one where annotation is pictorial.

Common Misconceptions:

- 1. Precision and accuracy are always misconceived as the tolerance of an apparatus and instrument. Many lay people always say that a burette is more precise than a measuring cylinder because it can measure more accurately. A science student, however, should say that a burette has a lower tolerance than a measuring cylinder.
- 2. Many students and teachers thought that beakers and conical flasks can be used to measure volumes. In reality, they are designed to hold liquids and the graduation scale at the side gives a very rough estimate of the volume of liquid that each of the flask holds. If a particular volume of a liquid, say, 100 ml, is to be measured, a measuring cylinder should be used.
- 3. Some students attached a percentage value, usually 5 %, to the criteria for accuracy. In reality, there is no such criterion. If the true value is 5.0 and the experimental value is 4.5 ± 0.5, then the percentage error is 10 %, but it is still accurate as 4.5 ± 0.5 encompasses the true value of 5.0. In Aspect 2 "evaluating procedure(s)" of "Conclusion and Evaluation" of Internal Assessment, students are asked to comment on the precision and accuracy of the measurements made. In this aspect, students will have to comment on the consistency of the measurements (precision) and whether the literature value is within the experimental value (accuracy). Students are also encouraged to determine the percentage error.

On a separate note, in the testing of drugs, researchers and statisticians use hypothesis testing and they allow only a 1% probability that the drug will not work or has side-effects. In the study of behaviours in human and animals, that interval is increased to 5%. Both figures apply to "two-tailed" tests. If it is a "one-tailed" test, the probability is halved. This has nothing to do with error determination. Students who are interested may read any statistics textbooks on t-testing, ANOVA and X²-testing.

Exercise 1

[Specimen HL Chemistry Paper (for first examinations in 2009)]

1. The following diagram shows a set of experimental data points, X, determined when one experimental measurement was repeated three times. The centre of the diagram represents the ideal value calculated from theory. What statement is correct about these measurements?



- A. The measurements involve low accuracy and low precision.
- B. The measurements involve low accuracy and high precision.
- C. The measurements involve high accuracy and low precision.
- D. The measurements involve high accuracy and high precision.

Answer: B

Accuracy refers to how close a measured value is to the correct value. The readings obtained, represented by 'X' are not in the centre of the diagram, indicating a deviation from the correct value. Therefore, the accuracy is low.

Precision indicates the closeness of agreement between independent test results obtained under stipulated conditions. The readings obtained are in close agreement of each other as they are clustered together in the same region. Therefore, precision is high.

 The data below is from an experiment used to measure the enthalpy change for the combustion of 1 mole of sucrose (common table sugar), C₁₂H₂₂O₁₁(s). The time-temperature data was taken from a data-logging software programme.

	A	В	С	D	E	F	G	н	1	J	K
1	Time (s)	Temperature (°C)									
2	0	23.03									
3	15	23.03									· · · · ·
4	30	23.07	1		DI	+ - 6 T					
5	45	23.19	1		P10	ot of 1	verst	IS I			
6	60	23.3]								[
7	75	23.36	220.	_							
8	90	23.43	23.0								
9	105	23.48	227.								
10	120	23.54		1			1				
11	135	23.57	326								
12	150	23.6	- 0.62]		-					
13	165	23.63	02.5		•						
14	180	23.64	25.5 -	1	•						
15	195	23.65			•						
16	210	23.66	0 23.4	1							
17	225	23.66	L 02.2		-						
18	240	23.67	23.3	1 •							
19	255	23.67									
20	270	23.69	23.2 -	1 •							
21	285	23.69									
22	300	23.7	23.1 -	1.							
23	315	23.7		÷-							
24	330	23.7	23 -	1							
25	345	23.7									
26	360	23.7	22.9 -					-	1		- [
27	375	23.7		0	100	20	0	300	400)	500 L
28	390	23.7		•			*	2			
29	40.5	23.7					£ (S)				[
30	420	23.7									[
31	435	23.7									
32											
33											
34											
35											
H 4	▶ ⊨ \ Sheet1	/ Sheet2 / Sheet3 /							<		

Mass of sample of sucrose, m = 0.4385 g

Heat capacity of the system, $C_{\text{system}} = 10.114 \text{ kJ K}^{-1}$

- (a) Calculate ΔT , for the water, surrounding the chamber in the calorimeter.
- $\Delta T = 23.7 23.03 = 0.67 \approx 0.7 \circ C (1 dp)$
- (b) Determine the amount, in moles, of sucrose.

Amount of sucrose = $\frac{0.4385}{(12.01 \times 12) + (22 \times 1.01) + (11 \times 16.00)} = \frac{1.282 \times 10^{-3} \text{ mol } (4 \text{ sf})}{(12.01 \times 12) + (22 \times 1.01) + (11 \times 16.00)}$

(c) (i) Using the following formula provided, calculate the enthalpy change for the combustion of 1 mole of sucrose.

$$Q = C_{system} \Delta T$$
 , $\Delta H = -\frac{Q}{n}$

$$Q = C_{system}\Delta T = (10.114) (0.7) = 7.0798 \approx 7 \text{ kJ} (1 \text{ sf})$$

$$\Delta H = -\frac{Q}{n} = -\frac{7}{1.282 \times 1.282^{-3}} = -5460 \text{ kJ mol}^{-1} \approx -5 \times 10^3 \text{ kJ mol}^{-1} \text{ (1 sf)}$$

Using the Data Booklet, calculate the percentage experimental error based on the (ii) data used in this experiment.

Experimental error

$$= \left| \frac{\text{Experimental value} - \text{Literature value}}{\text{Literature value}} \right| \times 100 \%$$

$$= \left| \frac{(-5000) - (-5640)}{(-5640)} \right| \times 100 \%$$

$$= 11.3 \% (3 \text{ sf})$$

[Specimen HL Chemistry Paper (for first examinations in 2016)] 3. Which combination in the table correctly states the value a

Which combination in the table correctly states the value and units of the gradient?



	Value	Units
A.	$\frac{3.0 \times 10^{-3} - 0.6 \times 10^{-3}}{0.050 - 0.010}$	S ^{−1}
B.	$\frac{3.0 \times 10^{-3} - 0.6 \times 10^{-3}}{0.050 - 0.010}$	S
C.	$\frac{0.050 - 0.010}{3.0 \times 10^{-3} - 0.6 \times 10^{-3}}$	S ^{−1}
D.	$\frac{0.050 - 0.010}{3.0 \times 10^{-3} - 0.6 \times 10^{-3}}$	S

Answer: A

Gradient =
$$\frac{y_2 - y_1}{x_2 - x_1} = \frac{3.0 \times 10^{-3} - 0.6 \times 10^{-3}}{0.050 - 0.010}$$

Units of gradient = $\frac{\text{mol dm}^{-3} \text{ s}^{-1}}{\text{mol dm}^{-3}} = \text{s}^{-1}$

Further reading:

- 1. Talbot, C.; Harwood, R.; Coates, C. Measurement and data processing. *Chemistry for IB Diploma.* Hodder Education: London, 2010; pp 303–325.
- 2. Bylikin, S.; Horner, G.; Murphy, B.; Tarcy, D. Measurement and data processing. 2014 Edition Chemistry Course Companion. Oxford University Press: Oxford, 2014; pp.261-276.
- 3. Analytical Methods Committee (September, 2003). Terminology the key to understanding analytical science. Part 1: Accuracy, precision and uncertainty. *AMC Technical Brief*. RSC, Cambridge

References:

- Jackson, H. Decimals Places & Significant figures https://www.brad.ac.uk/wimba-files/msucourse/media/DP%20and%20SF%20teaching.pdf (accessed Dec 25, 2017)
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