Topic 11: Measurement and data processing

10 hours

Essential idea: All measurement has a limit of precision and accuracy, and this must be taken into account when evaluating experimental results.

11.1 Uncertainties and errors in measurement and results

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

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?

Utilization:

- Crash of the Mars Climate Orbiter spacecraft.
- Original results from CERN regarding the speed of neutrinos were flawed.

Syllabus and cross-curricular links:
Option D.1—drug trials

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.

11.1 Uncertainties and errors in measurement and results

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.

Essential idea: Graphs are a visual representation of trends in data.

11.2 Graphical techniques	
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. **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? **Utilization:** • Graphical representations of data are widely used in diverse areas such as population, finance and climate modelling. Interpretation of these statistical trends can often lead to predictions, and so underpins the setting of government policies in many areas such as health and education. Syllabus and cross-curricular links: Topic 1.3—gas volume, temperature, pressure graphs Topic 6.1—Maxwell–Boltzmann frequency distribution; concentration–time and rate–concentration graphs Topic 16.2—Arrhenius plot to determine activation energy Topic 18.3—titration curves Option B.7—enzyme kinetics Option C.5—greenhouse effect; carbon dioxide concentration and global temperatures Option C.7—first order/decay graph **Aims:** • **Aim 7**: Graph-plotting software may be used, including the use of spreadsheets and the derivation of best-fit lines and gradients.

Essential idea: Analytical techniques can be used to determine the structure of a compound, analyse the composition of a substance or determine the purity of a compound. Spectroscopic techniques are used in the structural identification of organic and inorganic compounds.

11.3 Spectroscopic identification of organic compounds

Nature of science:

Improvements in instrumentation—mass spectrometry, proton nuclear magnetic resonance and infrared spectroscopy have made identification and structural determination of compounds routine. (1.8)

Models are developed to explain certain phenomena that may not be observable—for example, spectra are based on the bond vibration model. (1.10)

Understandings:

- The degree of unsaturation or index of hydrogen deficiency (IHD) can be used to determine from a molecular formula the number of rings or multiple bonds in a molecule.
- Mass spectrometry (MS), proton nuclear magnetic resonance spectroscopy (^{1}H NMR) and infrared spectroscopy (IR) are techniques that can be used to help identify compounds and to determine their structure.

Applications and skills:

- Determination of the IHD from a molecular formula.
- Deduction of information about the structural features of a compound from percentage composition data, MS, ^{1}H NMR or IR.

Guidance:

- The electromagnetic spectrum (EMS) is given in the data booklet in section 3. The regions employed for each technique should be understood.
- The operating principles are not required for any of these methods.

International-mindedness:

- Monitoring and analysis of toxins and xenobiotics in the environment is a continuous endeavour that involves collaboration between scientists in different countries.

Theory of knowledge:

- Electromagnetic waves can transmit information beyond that of our sense perceptions. What are the limitations of sense perception as a way of knowing?

Utilization:

- IR spectroscopy is used in heat sensors and remote sensing in physics.
- Protons in water molecules within human cells can be detected by magnetic resonance imaging (MRI), giving a three-dimensional view of organs in the human body.

Syllabus and cross-curricular links:
Topic 1.2—determination of the empirical formula from percentage composition data or from other experimental data and determination of the molecular formula from both the empirical formula and experimental data.

11.3 Spectroscopic identification of organic compounds	
• The data booklet contains characteristic ranges for IR absorptions (section 26), ^{1}H NMR data (section 27) and specific MS fragments (section 28). For ^{1}H NMR, only the ability to deduce the number of different hydrogen (proton) environments and the relative numbers of hydrogen atoms in each environment is required. Integration traces should be covered but splitting patterns are not required.	Topic 2.1—the nuclear atom Topic 5.3—bond enthalpies **Aims:** • **Aim 7**: Spectral databases could be used here. • **Aim 8**: The effects of the various greenhouse gases depend on their abundance and their ability to absorb heat radiation.