SL IB Chemistry

Your notes

Tool 2: Technology

Contents

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Applying Technology to Collect Data in Chemistry

- Computational chemistry is an advanced field that involves the use of computer simulations and theoretical methods to study chemical systems and investigate chemical reactions
- It also involves the use of computers to identify **trends** and make **predictions** from large **data sets**, for example of reactivity or molecular properties
- These large **data sets** can be collected experimentally for example, via the use of **sensors**, from existing **databases** or from **models** and **simulations**

Collecting data using data loggers and sensors

- Using a **data logger** and different **sensors** are essential in many scientific experiments for obtaining and analysing reliable results

Data loggers

- Data loggers are a tool that allows for the **quick and efficient gathering of data**
  - The information contained within a data logger can be inputted into a computer and formatted into a **table**
  - After this is done the computer is able to calculate the **average** and **plot graphs** using the data and calculate gradients quicker and more accurately than humans
- Data loggers are electronic devices that automatically monitor and record environmental parameters over time such as temperature, pressure, pH or conductivity
  - It can be connected to a variety of different sensors to receive the information and a computer chip to store it
  - Results are displayed on the data logger in real time

Use of a data logger and sensor

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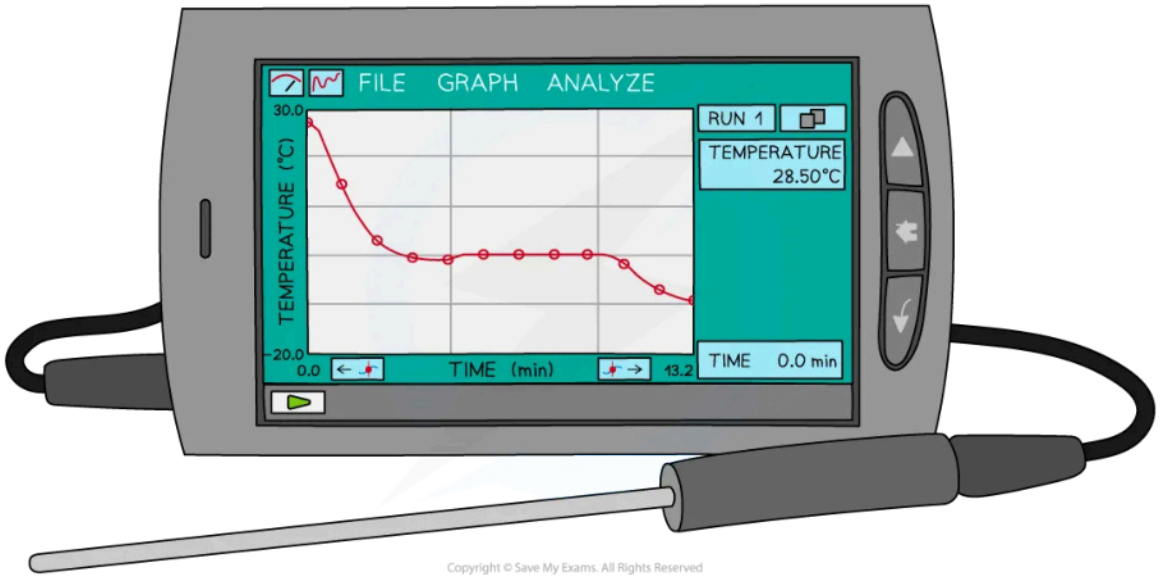


A data logger measuring and displaying temperature using a temperature probe

Sensors

- **Sensors** can be used to measure various **physical** and **chemical** properties of substances
- Sensors are **input** devices that detect and respond to specific changes in their surroundings, converting the detected information into electrical signals stored within the data logger
- Sensors allow chemists to easily collect large sets of data in a short space of time
- Here are some common types of sensors used in chemistry and how they can be applied:

pH meters

- pH meters measure the acidity or alkalinity of a solution expressed as a **pH value**
- A pH value is a measure of the concentration of **hydrogen ions** (H^+) in the solution
- A pH meter consists of two electrodes, one is a reference electrode and the other contains a special glass membrane that is sensitive to changes in the concentration of H^+ ions in the solution
- When the pH meter is immersed in the solution, the pH electrode's glass membrane interacts with the H^+ ions in the solution, the reference electrode provides a stable reference potential, and the pH meter measures the potential difference between the two electrodes
- Uses of pH meters include:
  - To determine the end point in acid-base titrations
  - To measure the pH of various solutions to study the behaviour of acids, bases, and salts in different chemical reactions
  - To study buffer solutions, for example, to monitor their effectiveness to resist changes in pH on small additions of acid or base

Temperature probes

- Temperature sensors are used to measure the temperature of a system or a reaction

- They are crucial for carrying out experiments that require specific temperature conditions or monitoring exothermic/endothermic reactions
- Temperature sensors can be used instead of thermometers in practical investigations and enable
- For examples of investigations where temperature is measured, see our revision notes on Calorimetry Experiments

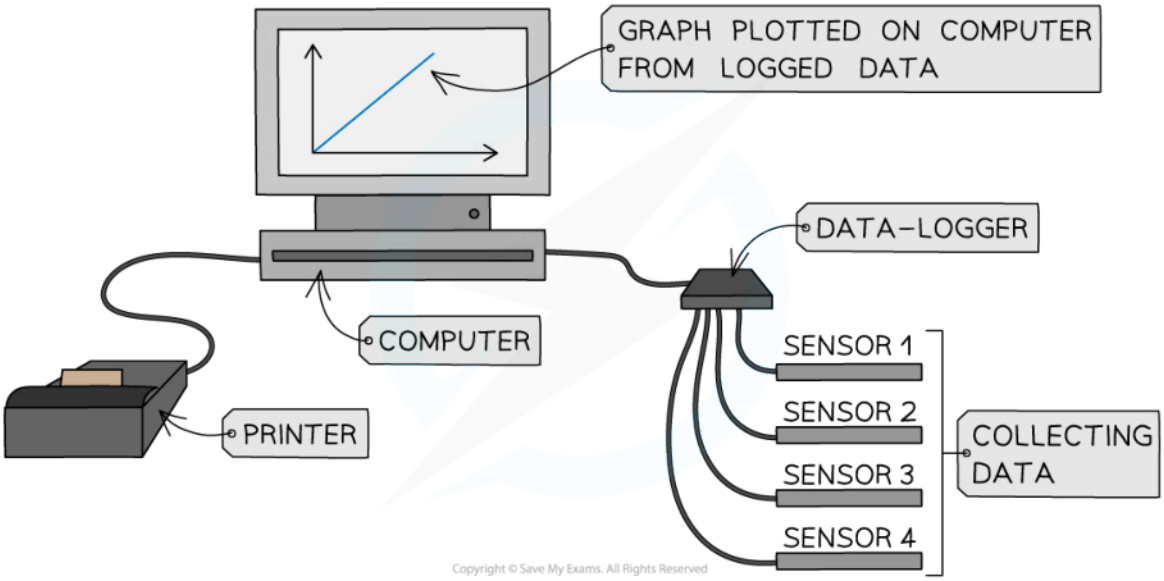
Pressure sensors

- Pressure sensors measure the pressure of gases or liquids
- In chemistry, they can be used in gas law experiments or to monitor changes in pressure during chemical reactions

Conductivity sensors

- Conductivity sensors measure the electrical conductivity of a solution, which is related to the concentration of ions present
- They are commonly used to determine the concentration of ions in a solution or to study the behaviour of electrolytes
- The changes in the conductivity of a reaction mixture can be used to determine the rate of reaction
- For more information on using conductivity to determine the rate of a reaction, see our revision notes on Measuring Rates of Reaction

Data logging in chemistry



Data logging is a useful part of the chemist's laboratory toolkit

Identifying and extracting data from databases

- A database is a **structured collection of data** so it can be searched**, sorted, filtered** and **analysed** quickly
  - Data in a database can be any type of data including text, images, videos, sound
- Databases that you may come across during your studies include:

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- Formulae of polyatomic ions, used to write formulae of compounds containing the ion and equations
- Physical properties, e.g. melting points, boiling points
- Thermodynamic data such as enthalpy values, entropies, Gibbs energy values
- Kinetic data, such as rate constants
- Equilibrium constants
- Spectroscopic data, such as NMR and IR spectra
- Chemical structures and properties
- Organic synthesis information, including reaction conditions and procedures for the preparation of specific organic compounds
- Bond lengths

- This is by no means an exhaustive list

Useful websites for databases

- The Spectral Database for Organic Compounds - contains a range of information about a compound including molecular formulae, weight, atomic structure, spectra (13C NMR, 1H NMR, IR)
- MolCalc - provides a 3D molecule of different molecules and gives a range of their properties including enthalpy values, heat capacity, entropy, vibrational frequencies, molecular orbitals and polarity
- PubChem - a large database containing lots of information about over 700,000 chemicals including 2D and 3D structures, names, chemical and physical properties
- ChemSpider - includes chemical properties and spectra
- NIST WebBook - includes formulae and properties and also allows you to search for reactions

Generating data from models and simulations

- A **model** is a **simplified** version of reality
  - For example, the ball-and-stick model is a three-dimensional model which represents compounds, using balls to represent atoms and sticks to represent chemical bonds, giving us a visual representation of the structure and bond angles within compounds
- Models in chemistry are often used to represent and explain various phenomena, structures, and interactions at the atomic and molecular level
  - The model can then be **analysed** or **tested** to learn more about how the system works and to **predict** how the system might **respond** to change
- Some models can be very **simple**, such as a child's model car, whilst other models can be **highly complex** and require the power of supercomputers, such as the computer models that are currently being used to predict how our climate will change in the future
  - To some extent, due to their very nature, all models involve some level of **approximation** or **simplification**, and therefore some loss of accuracy (even the very powerful and complex models)
- Chemists also use **simulations** which use models based on the fundamental principles of chemistry to predict the behaviour of atoms, molecules and chemical systems
- Simulations are a valuable tool to be able to explore scenarios that may not be feasible or safe to investigate in a physical laboratory
  - For example, to predict the reactions between Group 1 metals towards the bottom of the group with water which are dangerously vigorous based on models of the reactions of other Group 1

metals with water

- The **accuracy** and **reliability** of the simulation depend on the quality of the models and assumptions used to create them
- Simulations allow you to alter variables in a particular scenario and allow you see to the effect of these changes, for example:
  - Simulations of gas particles allow you to explore how gases behave
  - The simulation uses models of gas laws to predict how the system will respond to changes in temperature, pressure and volume which are controlled by the user
  - Data can be collected from these predictions of behaviour

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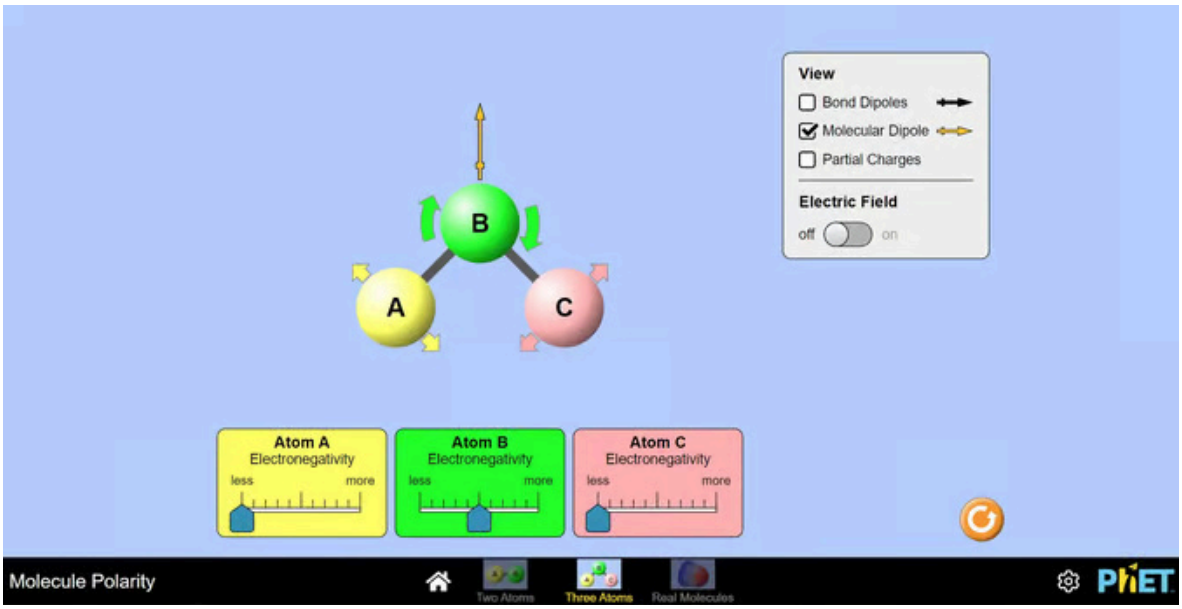
The PhET Simulations Website



There is a range of online resources that allow you to run simulations of chemical phenomena, a particularly useful site is PhET, which includes simulations of molecule shapes, the pH scale and states of matter

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Applying Technology to Process Data in Chemistry

- Data plays a crucial role in understanding chemical processes, conducting experiments, and making informed decisions
- As the volume and complexity of data continue to grow, the integration of technology has become essential for efficiently processing, analysing and interpreting chemical data
- Using technology to process data can be demonstrated when conducting your internal assessment as well as during practical investigations where you should look for opportunities to:
  - Use spreadsheets to manipulate data
  - Represent data in a graphical form
  - Use computer modelling

Using Spreadsheets to Manipulate Data:

- Spreadsheets are versatile and widely used for data manipulation, organisation, and analysis in chemistry

Data Organisation:

- Allows you to efficiently input raw data, categorise it by parameters and organise it into columns and rows
- Allows you to simplify data navigation and understanding

Data Manipulation:

- Allows you to perform various calculations, statistical analyses and mathematical operations on datasets effortlessly
- It is useful for processing experimental results and deriving meaningful conclusions

Data Visualisation:

- Spreadsheets employ built-in functions and formulas to automatically generate graphs and charts
- Visualise trends, patterns, and correlations in the data, facilitating quick insights
- For example, plotting data on spreadsheets can quickly enable you to produce graphs and spot patterns and trends, such as graphs of:
  - First ionisation energy for elements against atomic number
  - pH against the volume of acid during neutralisation

Using spreadsheets to create graphs

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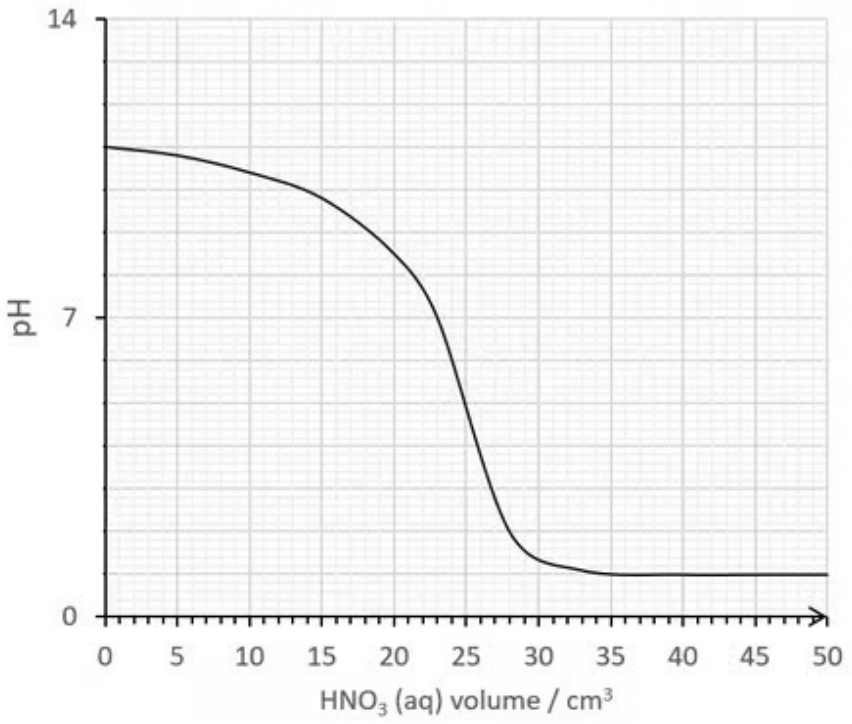
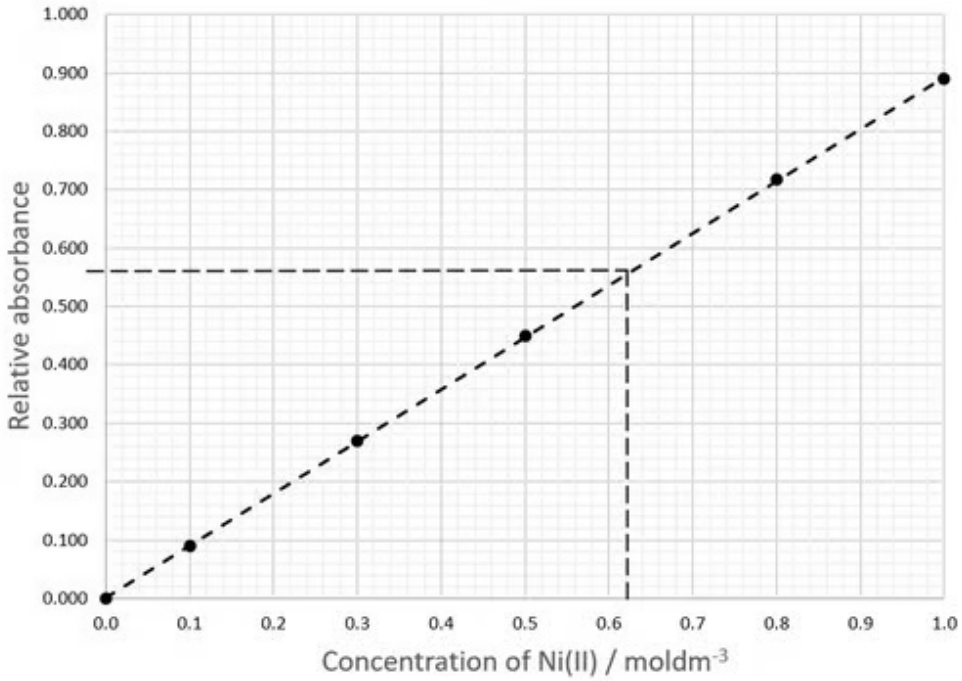


Recording the output from a digital pH probe directly into a spreadsheet can enable you to quickly plot graphs and identify trends

Representing Data in a Graphical Form:

- Graphical forms of representations offer the following advantages:
  - Graphical representation simplifies complex data
  - Line graphs and scatter plots reveal trends and correlations
  - Bar graphs and pie charts facilitate data comparison
  - Molecular structure diagrams and 3D models offer insights into chemical systems

Sample Calibration Curve



A line graph of absorbance against concentration is essential for correlating the output of a colorimeter against the concentration of known standard solutions. This is known as a calibration curve and can be used in kinetics investigations. The dotted tie lines shown how the concentration of an unknown solution can be found from the absorbance

Chemistry and Modeling:

- Computational models help gain insights into complex chemical processes, saving time and resources compared to purely experimental approaches

Molview 3D modelling software

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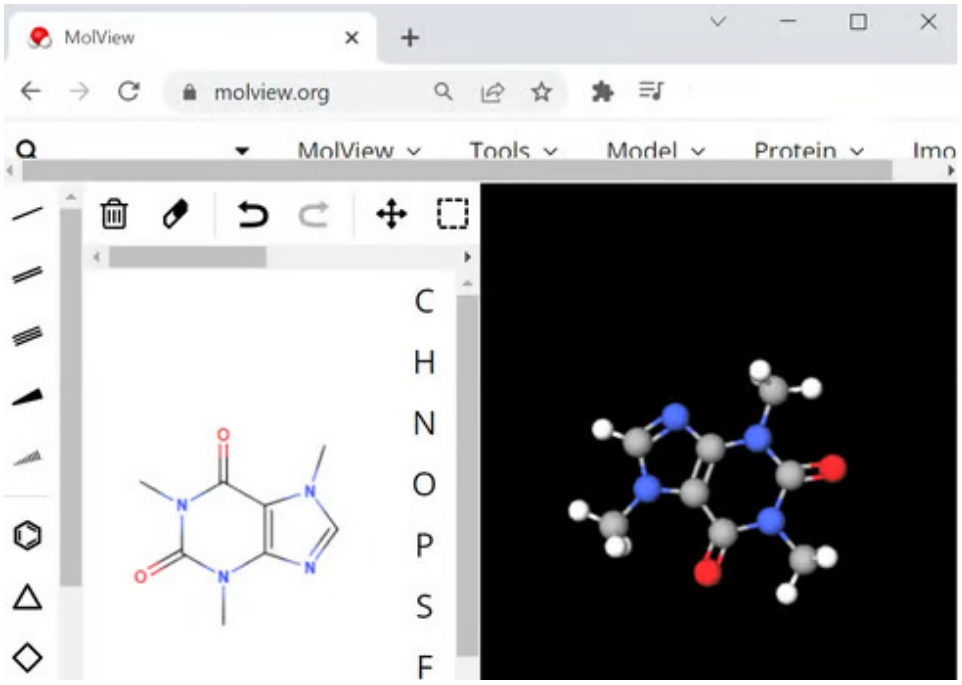

Molview is a free 3D visualisation aid which you can quickly build your own structures and see what they look like in 3D

Visualisation Tools:

- Data visualisation tools play a crucial role in presenting complex chemical data in an accessible and understandable format
- Interactive 3D visualisation software such as molview aids in exploring molecular structures, facilitating a better understanding of their behaviour and interactions
- Graphical representations of reaction pathways and kinetic data assist in elucidating reaction mechanisms

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