1.2 The mole concept

Nature of science:

Concepts—the concept of the mole developed from the related concept of "equivalent mass" in the early 19th century. (2.3)

Understandings:

- The mole is a fixed number of particles and refers to the amount, *n*, of substance.
- Masses of atoms are compared on a scale relative to ^{12}C and are expressed as relative atomic mass (A_r) and relative formula/molecular mass (M_r).
- Molar mass (M) has the units g mol^{-1}.
- The empirical formula and molecular formula of a compound give the simplest ratio and the actual number of atoms present in a molecule respectively.

Applications and skills:

- Calculation of the molar masses of atoms, ions, molecules and formula units.
- Solution of problems involving the relationships between the number of particles, the amount of substance in moles and the mass in grams.
- Interconversion of the percentage composition by mass and the empirical formula.
- Determination of the molecular formula of a compound from its empirical formula and molar mass.
- Obtaining and using experimental data for deriving empirical formulas from reactions involving mass changes.

Guidance:

- The value of the Avogadro's constant (L or N_A) is given in the data booklet in section 2 and will be given for paper 1 questions.
- The generally used unit of molar mass (g mol^{-1}) is a derived SI unit.

International-mindedness:

- The SI system (Système International d'Unités) refers to the metric system of measurement, based on seven base units.
- The International Bureau of Weights and Measures (BIPM according to its French initials) is an international standards organization, which aims to ensure uniformity in the application of SI units around the world.

Theory of knowledge:

- The magnitude of Avogadro's constant is beyond the scale of our everyday experience. How does our everyday experience limit our intuition?

Utilization:

- Stoichiometric calculations are fundamental to chemical processes in research and industry, for example in the food, medical, pharmaceutical and manufacturing industries.
- The molar volume for crystalline solids is determined by the technique of X-ray crystallography.

Syllabus and cross-curricular links:
Topic 2.1—the scale of atoms and their component particles
Topics 4.1, 4.3 and 4.5—lattice structure of ionic compounds, molecular structure of covalent compounds and metallic lattice
Topics 5.1 and 15.2—standard enthalpy and entropy changes defined per mole
Topic 19.1—mole ratios of products in electrolysis

Aims:

- **Aim 6**: Experiments could include percent mass of hydrates, burning of magnesium or calculating Avogadro's number.
- **Aim 7**: Data loggers can be used to measure mass changes during reactions.

UNIT 1.2 – THE MOLE CONCEPT

One Mole (mol): The same as saying one dozen of something but instead of 12 it is 6.02×10^{23}

Avogadro's Constant: 6.02×10^{23}

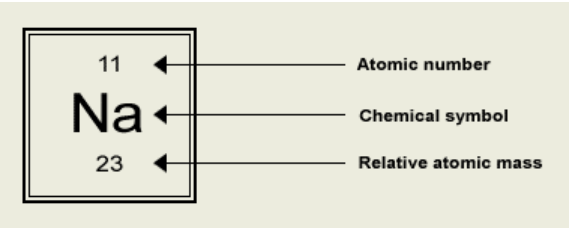
This is the number of atoms in exactly twelve grams of the isotope carbon-12 ($^{12}_{6}C$)

Eg. How many atoms of hydrogen are there in 1.00 mol of methanal (HCHO) molecules?

Answer: 1.20×10^{24} (Because 2 times Avogadro's constant equals that)

RELATIVE ATOMIC MASS

Relative Atomic Mass (A_r): The weighted average mass of one atom of an element relative to one-twelfth of an atom of carbon-12.



RELATIVE ISOTOPIC MASS

Relative Isotopic Mass (I_r): The relative mass of each isotope ion naturally occurring element.

Measured relative to carbon-12

Shown in mass spectrometer tables.

RELATIVE FORMULA MASS

Relative Formula Mass (M_r): The combination of all A_r values in the molecule.

Also known as Molar Mass: The mass of one mole of a substance (g mol^{-1})

H_2O

H=1 O=16

(1x2)+16=18

MOLE CALCULATIONS

$$Moles\ of\ atoms = \frac{mass}{A_r}$$

$$Moles\ of\ compounds = \frac{mass}{M_r}$$

$$Number\ of\ particles = Moles * Avogadro's\ Constant$$

EMPIRICAL FORMULAS

Empirical formula of a compound: The simplest whole number ratio of the elements present in one molecule or formula unit of the compound.

Molecular formula of a compound: Shows the actual number of atoms of each element present in a molecule.

How to calculate percentage by mass:

"Calculate the percentage by mass of sulphur in sulphuric acid, H_2SO_4."

$$\%\ Sulfur = \frac{A_r(S)}{M_r(H_2SO_4)} * 100\%$$

$$= \frac{32.07}{2(1.01) + (32.07) + 4(16.00)} * 100\%$$

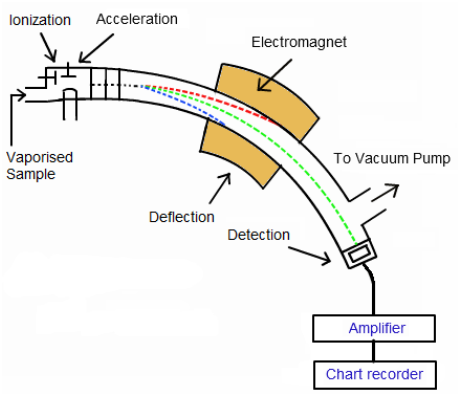
$$= 32.69\%$$

If given the percentage by mass of an element in a molecule, the empirical formula can be found.

	Si	*O*
Percentage by Mass	47%	100 – 47 = 53%
Mass in 100 g	47 g	53 g
Molar Mass	28 g/mol	16 g/mol
Number of moles	1.68 mol	3.31 mol
Simplest Ratio	1	2
	SiO_2	

MASS SPECTROMETRY

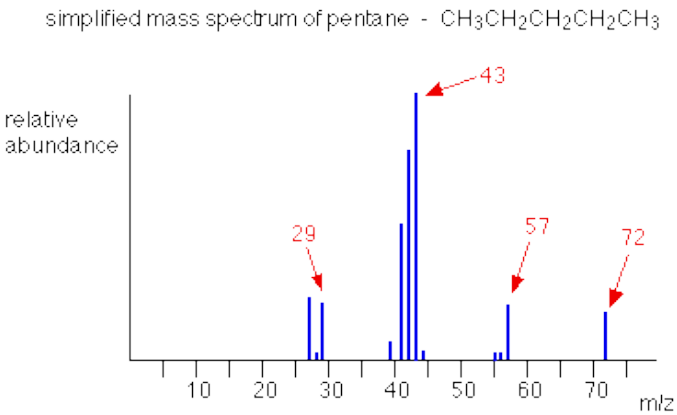
An analytical chemistry technique that helps identify the amount and type of chemicals present in a sample by measuring the **mass-to-charge** ratio and abundance of gas-phase ions. A **mass spectrum** is a plot o the ion signal as a function of the **mass-to-charge** ratio.



How it works:

1. Liquids and solids are **vaporised**
2. Spare electrons are hurled at the sample to knock of electrons (**ionize**), making the sample cations
3. A strong electric field **accelerates** the ions
4. Magnetic fields **deflect** the ions according to their mass (heavier ones are deflected the least)
5. Electronic **detection** detects the abundance of each ion
6. The data is then recorded as a **mass spectrum**

MASS SPECTRUM



Graphs the mass:charge (Relative Isotomic Mass) against the relative abundance.

Sometimes more than one electron is knocked off during **ionization** creating a 2+ positive charge. This explain the small peaks that sometimes occur in the mass spectrum. We divide the mass at that point by 2.

CALCUALATIONS

$$A_r = \sum \frac{(I_r * \%Abundance)}{100}$$