1.1 Introduction to the particulate nature of matter and chemical change

Particle Nature of Matter

- Matter is anything that takes up space
- Matter can either refers to the particles (pure substances) or combination of a substances (mixtures):

Pure Substances

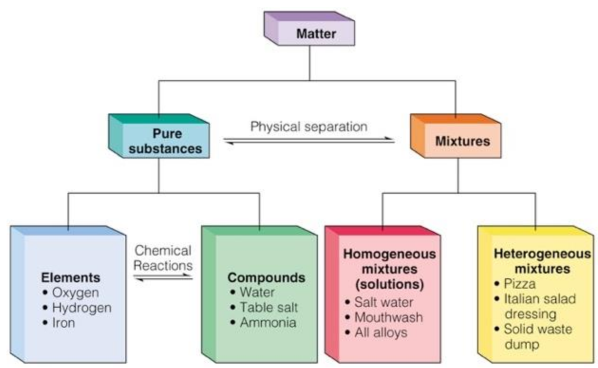
- A pure substance has definite and constant composition
- For a pure substance, from a particle perspective all particles will look and remain the same

Definitions
Element – Atoms all having the same number of protons **Molecule** – Two or more elements chemically join together **Compounds** – Two or more different elements chemically joined together in a fixed ratio

- From their definitions: All compounds are molecules, but not all molecules are compounds
- When the elements are joined, the atoms lose their individual properties and have different properties from the elements they are composed of

Mixtures

- Mixture: A combination of pure substances
- Mixtures contain more than one element and/or compound that are not chemically bonded together, so retain their individual properties
- Mixtures are either homogeneous or heterogeneous:
- Homogeneous mixtures are the same mixture throughout
    - They will have a <u>uniform composition</u>
- Heterogeneous mixtures have a different mixture throughout
    - They will have <u>visibly different substances or phases throughout, a non-uniform composition</u>

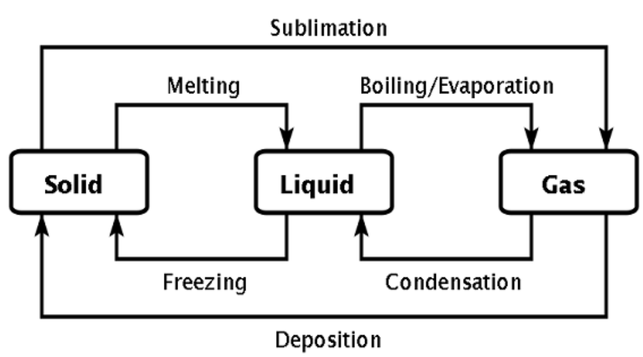


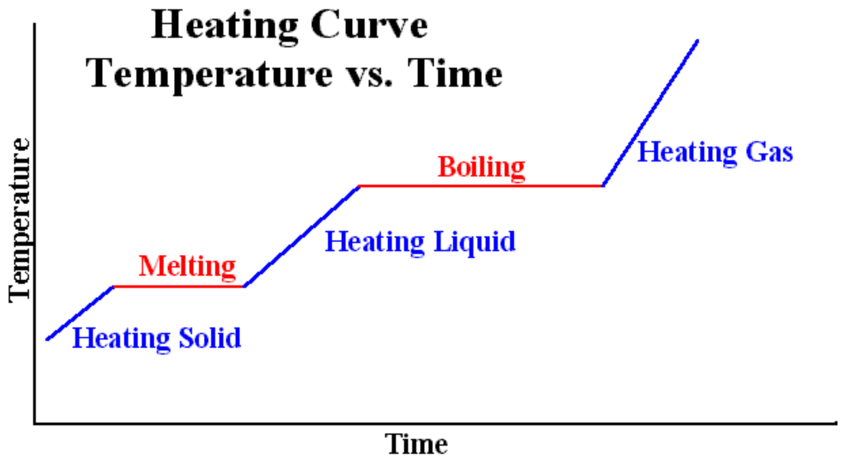
Chemical Equation

- Chemical Equation: Describes what happens during a chemical reaction
- A chemical reaction will always have reactants and products as well as some special reaction conditions if required
- Reactants are always on the left, and products are always on the right: $Reatants \rightarrow Products$
- Chemical equations usually use state symbols to identify the state of the products and reactants

State Symbols

- Reactants and products can be in one of four states
    - (s): solid
    - (l): liquid
    - (g): gas
    - (aq): aqueous solution (dissolved in a solvent)
- The changes of state are to the left:
- A heating curve is a graph showing the temperature of a substance plotted against the amount of energy it has absorbed





- **Note, during a state change there will be no increase or decrease in temperature**
- Adding temperature only increases the kinetic energy of the molecules, which will eventually break the bonds, then the molecules will change state
- It also takes a higher temperature to turn a solid to a liquid, and an even greater temperature to turn a liquid to a gas

Physical and Chemical Changes

- **In a physical change, no new substances are produced**
  - Example: The melting of ice is a physical change. It is being changed physically
- **In a chemical change, new chemical substances are formed**
  - The atoms in the reactants are rearranged to form new products. It is being changed chemically

1.2 The mole concept and Avogadro's Constant

The Mole

Definitions
Mole – The amount of substance that contains the same number of specified particles as there are atoms in 12g of Carbon-12

- When dealing with particles of the size of atoms and molecules, it becomes very difficult to do the calculations as they are present in very large numbers. So to make these calculations simpler, answers are expressed in mol
- The mole is given by the symbol n
- The mole makes it possible to correlate the number of particles with the mass that can be measured
- The number of particles in 1 mole is given by Avogadro's constant
  - Avogadro's constant (L): **1 mol = 6.02 x 10^{23} particles (atoms, molecules, ions)**
- In order to calculate number of particles: $N = n \times L$
  - N: number of particles (atoms, molecules, ions)
    - Atoms are simple elements, ions are elements with a charge, and molecules are more than one atom
  - n: number of moles
  - L: Avogadro's number
- We can also rearrange this formula if we want to find number of mols: $n = \frac{N}{L}$

Mole question:

Calculate the number of O_2 molecules in 1.5 mol of oxygen (O_2)

$n(O_2) = 1.5mol$

$L = 6.02 \times 10^{23}$

Therefore: $N = n \times L => N = 1.5 \times 6.02 \times 10^{23} = 9.0 \times 10^{23}$

Mole relationships

- A chemical formula shows the mole relationship between the individual atoms that make up that molecule. Example:
    - Methane gas is produced from the combination of 1 mol of carbon atoms and 4 mol of atoms
    - 1 mol of C + 4 mol of H → 1 mol of CH_4
- To find the number of mol of an element in a molecule multiply the number of that element in the molecule by the amount of mol of that molecule:

$$n(X) = \# \times amount\ of\ mols$$

- To find the number of atoms of an element in a molecule multiply the above equation by L
- To find the total number of atoms of a molecule multiply the amount in mol by the number of atoms in the molecule

Mole relationship question:

1. Calculate the number of mol of oxygen in 0.05 mol of O_2 molecules

$N(O) = 2 \times n(O_2)$ *note that there is a two because in one molecule of O_2 there are two oxygen atoms ratio ∴ is 2:1*

$N(O) = 2 \times 0.05$

$N(O) = 0.1mol$

2. Calculate the number of mol of SO_4^{2-} ions in a 2.39×10^{-3} mol sample of $PbSO_4$

$n(PbSO_4) = 2.39 \times 10^{-3}$

$n(SO_4{}^{2-}) = n(PbSO_4)$ *It is equal because the ratios are equal*

$n(SO_4{}^{2-}) = 2.39 \times 10^{-3}$

The Mole Concept

- Masses of atoms are compared on a scale relative to ^{12}C and are expressed as relative atomic and molecular mass

Definitions

Relative atomic mass (A_r) – The <u>average</u> mass of all isotopes of an element compared to $\frac{1}{12}$ the mass of C_{12} atom

Relative molecular/formula mass (M_r) – <u>The mass of a molecule</u> compared to $\frac{1}{12}$ the mass of C_{12} atom

- The relative molecular mass (M_r) also called the molar mass can be calculated from its chemical formula using the relative atomic masses (A_r) of the elements from the periodic table
- Some elements will have a greater atomic mass than others despite their atomic number because they will either <u>have a greater proportion of heavier isotopes</u> or <u>they will have a greater number of neutrons</u>
- Relative atomic and molecular mass are **relative therefore it has no units**
- Molar mass (M) has the units g mol^{-1}

Relative molecular mass question:

Calculate the relative formula mass (molar mass) of Vitamin C: $C_6H_8O_6$

$M_r(Vitamin\ C) = [6 \times A_r(C)] + [8 \times A_r(H)] + [6 \times A_r(O)]$ *Note the multiples because there is a # of atoms*

$M_r(Vitamin\ C) = (6 \times 12) + (8 \times 1) + (6 \times 16)$

$M_r(Vitamin\ C) = 176$

Therefore $M_r(Vitamin\ C) = 176 gmol^{-1}$

Amount of moles

- In order to calculate number of moles: $n = \frac{m}{M}$ where
  - n: moles
  - m: mass
  - M: molar mass

Number of moles question:

Calculate the amount in mol of 1.2g of Nitric Oxide (NO)

$m = 1.2 \quad M = 14 + 16 = 30$

Therefore, since $n = \frac{m}{M} \rightarrow n = \frac{1.2}{30} = 0.04\ mol$

Percentage Composition

- The values of molar masses of elements in compounds can be used to calculate the % compositions of a compound once its formula is known
- This is given by the following equation:

$$\%\ composition\ by\ mass\ of\ element = \frac{molar\ mass\ of\ x}{molar\ mass\ of\ the\ compound}$$

Question: Determine the % composition by mass of each element in potassium nitrate (KNO_3)

$\%K = \frac{39.10}{101.11} \times 100 = 38.67\%$ $\quad \%O = \frac{3 \times 16.00}{101.11} \times 100 = 47.47\%$

$\%N = 100 - 38.67 - 47.47 = 13.86\%$

Empirical formula

- Empirical formula: The formula of a compound that shows the <u>lowest whole number</u> ratio of each type of atom
- To calculate the empirical formula of compounds we:
  1. Write the elements present in the compound
  2. Write each elements % composition or mass
  3. Divide the % or mass by the relative atomic mass and calculate the ratio
  4. Divide each ratio by the smallest ratio above to get a whole number ratio
  5. Express as an empirical formula

Question: A compound consists of carbon 75% and hydrogen 25% by mass. Determine empirical formula

$$C : H$$

$$\frac{75}{12.01} : \frac{25}{1.01}$$

$$\frac{6.24}{6.24} : \frac{24.8}{6.24}$$

$$1 : 4$$

Molecular formula

- Molecular formula: The formula of a compound that shows the actual number of each type of atom in the molecule
- A molecular formula gives the actual number of different atoms covalently bonded in one molecule
- The molecular formula is always a whole multiple of the empirical formula
- A molecular formula can be found is the molar mass is known

Question: Work out the molecular formula of CH_2 ($M_r = 70$)

$$Empirical\ Formula: A_r(C) + A_r(H_2) = 12 + 2 = 14$$

$$70 \div 14 = 5$$

$$CH_2 \times 5 = C_5H_{10}$$

Atom Economy

- The atom economy of a chemical reaction is a measure of the amount of starting materials that become useful products
- A high atom economy means that less waste is created and the reaction has a higher efficiency
- To calculate:

$$Atom\ economy = \frac{total\ mass\ of\ desired\ products}{total\ mass\ of\ all\ products/reactants} \times 100$$

1.3 Reacting masses and volumes

Limiting/Excess reactants

- Reactants can either be in limiting or excess:
  - The limiting reactant is the reactant that will be used up first in a chemical reaction
  - The excess reactant is the reactant that will be left over after the limiting reactant is used all up
- In order to determine limiting reactant, **divide the moles by the leading coefficient**
- The reactant with the lower number of moles is the limiting reactant

Question:

Sulfur hexafluoride (SF6) is a colorless, odorless, and extremely stable compound. It is formed by burning sulfur in the atmosphere of fluorine. Suppose that 4 moles of S are added to 20 moles of F_2. Which will be the limiting reagent?

$$S + 3F_2 \rightarrow SF_6$$

$n(s) \div 1 = 4\ mol\ \div 1 = 4$ *Divided by 1 because coefficient is one*

$n(F_2) \div 3 = 20\ mol\ \div 3 = 6.67$ *Divided by 3 because coefficient is three*

Therefore, S is limiting and F_2 is in excess

Percentage yield

- Experimental yield can be different from theoretical yield. The yield of a reaction is the actual mass of product obtained:
  - Some of the reactants may remain unreacted when the reaction is complete
  - Some of the product may be lost when liquids or solids are transferred from one container to another

- Some of the reactants may form other products

- A percentage yield is the amount of product produced experimentally compared to the theoretical amount
- In order to calculate percentage yield:

$$Percentage\ yield\ (\%) = \frac{actual\ yield}{theoretical\ yield} \times 100$$

Question:

10.00g of ethane (C_2H_4) will react with exactly 56.95g of bromine. The theoretical yield for this reaction is 66.95. The experimental yield of $C_2H_4Br_2$ prepared in an experiment was 50.00g. Calculate the percentage yield.

$$Percentage\ yield\ (\%) = \frac{actual\ yield}{theoretical\ yield} \times 100$$

$$\frac{50}{66.95} \times 100 = 74.68\%$$

Therefore, percentage yield if 74.68%

Theory of an ideal gas

- The kinetic molecular theory is a model used to explain the behavior of gases. The essential ideas are:
  - Gaseous particles are in continuous random motion, in straight lines not curved
  - Perfect elastic collision
  - Average kinetic energy is directly proportional to temperature
  - Volume of gas is negligible
  - No intermolecular forces (no attraction between particles)
- Note that no gas is perfectly ideal

Ideal Gas Equation

- Ideal gas equation: $PV = nRT$ where:
  - P: Pressure in kilopascals (kPa) *In IB convert to Pa*
  - V: Volume decimeters cubed (dm^3) *In IB convert to m^3*
  - n: Number of moles
  - T: Temperature in kelvin
  - R: 8.31 (Universal gas constant)

Question:

0.25 mol of nitrogen is placed in a flask of volume 5.0dm^3 at a temperature of 5°C. What is the pressure?

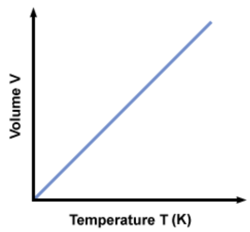
$P = x, V = 5.0\ dm^3, n = 0.25\ mol, T = 278K, R = 8.31$

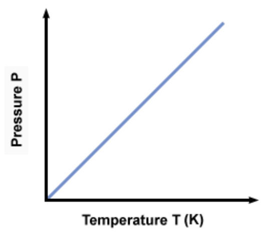
Therefore: $P(N_2) = \frac{nRT}{V} = \frac{0.25 \times 8.31 \times 278}{5.0} = 116kPa$

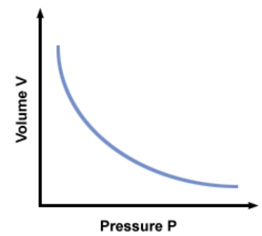
Combined Gas Equation

- The three gas laws applied to a fixed mass of gas can be summarized:
  - $P \propto \frac{1}{V}$ at constant temperature
  - $V \propto T$ at constant pressure
  - $P \propto T$ at constant volume
- These three laws can combine to form the combined gas law: $\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$

Law	Result	Formula
Combined gas law	$\frac{PV}{T} = k$	$\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$
Gay-Lussacs' law	$\frac{P}{T} = k$	$\frac{P_1}{T_1} = \frac{P_2}{T_2}$
Boyles' law	$PV = k$	$P_1V_1 = P_2V_2$
Charles's law	$\frac{V}{T} = k$	$\frac{V_1}{T_1} = \frac{V_2}{T_2}$







- An ideal gas will have the greatest volume at a high temperature and low pressure

Question:

A balloon has a volume of 150L at a pressure of 101kPa and a temperature of 27°C. It rises to an altitude of 15km where the temperature is -30°C and the pressure 12kPa.

What is the volume of the balloon at this altitude

$V_1 = 150L \quad V_2 = x$

$P_1 = 101kPa \quad P_2 = 12kPa$

$T_1 = 27 + 273K \quad T_2 = -30 + 273K$

Therefore: $V_2 = \frac{P_1V_1T_2}{T_1P_2} = \frac{101\times150\times(273+27)}{(273-30)\times12} = 1559L$

Real vs Ideal Gases:

- A gas behaves more like an ideal gas at a high temperature and lower pressure:
  - High temperature: The potential energy due to intermolecular forces becomes less significant compared with the particles kinetic energy
  - Low pressure: The size of the molecules becomes less significant compared to the empty space between them

Real Gases	Ideal Gases
Gas particles have volume	Gas particles do not have volume
Particles have attractive forces	No attractive forces between particles

Molar Volume

- The molar volume of an ideal gas is a constant at specified temperature and pressure
  - Molar volume (V_m): The volume occupied by one mole of a substance (chemical element or chemical compound) at a given temperature and pressure
- Avogadro's law states 1 mol of any gas at STP will occupy 22.7dm^3
  - Standard temperature and pressure (STP) conditions are at **273K** and **100kPa**

- Avogadro's law enables the mole ratio of reacting gases to be determined from volumes of the gases

$$n = \frac{V_m}{V}$$

- In order to calculate the volume of a gas at STP: $V = n \times V_m$
  - Where n: moles, V: volume of gas, V_m: molar volume of gas at STP

Question:

Determine the volume occupied by 16.g of oxygen gas (O_2 at STP)

$$n = \frac{m}{Mr} = \frac{16}{32} = 0.55$$

$$V(O_2) = n \times V_m = 0.500 \times 22.7 = 11.4$$

Molar Concentrations

Definitions

Solute – The smallest component in a solution (what is being dissolved)

Solvent – The largest component of a solution (what is it being dissolved in) (Remember VENT)

Solution – The solute and solvent combined (A homologous mixture)

Concentration – A measure of solute (mol) per solution (dm^{-3})

- Concentration can be calculated by: $concentration = \frac{mole\ of\ solute}{volume\ of\ solution} = \frac{n}{V}$

Question:

What is the concentration of sodium chloride in a saline solution if 200cm^3 of the solution contains 0.010mol NaCL

$c = \frac{n}{v} = \frac{0.010}{200/1000} = 0.050M(mol\ dm^{-3})$ *Volume is divided because dm^3 is needed*

Addition of solutions

- Calculate the new amount of mols by adding the number of moles from each individual solution, then find the new volume

Question:

Calculate the final concentration of mol dm^{-3} of $CaCl_2$ when 25cm^3 of 0.40M $CaCl_2$ added to 50cm^3 of 1.2M $CaCl_2$

$n(CaCl_2) = c \times v$	$n(CaCl_2) = c \times v$
$n(CaCl_2) = 0.40 \times 0.025$	$n(CaCl_2) = 0.40 \times 0.050$
$n(CaCl_2) = 0.010mol$	$n(CaCl_2) = 0.060mol$

Therefore, by adding both mols together we get 0.070mol. Now we need to calculate concentration:

$[CaCl_2] = \frac{n}{v} = \frac{0.070}{0.075} = 0.93M$

Dilution

- Dilution: The process of adding more solvent to a solution
- When a solution is diluted, the solute particles are more widely spread. There is a direct relationship between volume and concentration
- The dilution formula is then: $C_1V_1 = C_2V_2$

Question:

Calculate the molarity of $CaCl_2$ in 200cm^3 of 0.40M $CaCl_2$ diluted to 400cm^3 of water

$C_1 = 0.40M$ $\quad C_2 = x$ $\quad V_1 = 200cm^3$ $\quad V_2 = 400cm^3$

Therefore: $C_2 = \frac{C_1V_1}{V_2} = \frac{0.40 \times 0.200}{0.40} = 0.20M$