Stoichiometry

The story so far…

- The structure of an atom – protons, neutrons & electrons
- Electron structure & the Periodic Table
- Shapes of electron orbitals (Quantum Numbers)
- Essential and toxic elements – quantity & availability

The next topic: Stoichiometry & mole calculations

- Recap of the mole concept and balancing equations
- Calculations involving moles
- The ideal gas equation
- Partial pressures

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Mole Concept

- One mole is the number of atoms in exactly 12.0 g of the pure isotope carbon-12
- Avogadro's number (N_A) is the number of atoms/ions/molecules in one mole (6.022×10^{23})

$$\text{No of moles} = \frac{\text{Mass (g)}}{\text{Molar mass (g mol}^{-1})}$$

Significance:

- Easy to measure mass; but can not determine number of atoms/molecules directly.
- All reactions depend on *ratios* of reacting atoms/molecule.

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Balancing Chemical Equations

An equation is a quick way to represent a reaction

- Correct formula of all reactants & products
- Correct ratio of reacting species
- Balance of type & number of each element
- Indication of state (solid, liquid, gas, aqueous)
- May indicate conditions over the arrow

e.g. metabolism of glucose

$$C_6H_{12}O_6\,(aq) + 6\,O_2\,(g) \xrightarrow{\textit{in vivo}} 6\,CO_2\,(g) + 6\,H_2O\,(l)$$

+ energy

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Balance These Equations

1. Anaerobic fermentation of glucose ($C_6H_{12}O_6$) to form ethanol (C_2H_5OH) and carbon dioxide.

$$C_6H_{12}O_6\,(aq) \longrightarrow 2C_2H_5OH(aq) + 2CO_2(g)$$

2. Combustion of butane (C_4H_{10}) to form carbon dioxide and water.

$$2C_4H_{10}\,(g) + 13O_2\,(g) \longrightarrow 8CO_2(g) + 10H_2O(l)$$

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Calculations involving moles

e.g. Converting mass to moles n=m/M

- How many moles of glucose are in 10.0g?

Molar mass of $C_6H_{12}O_6$ is (6x12.01)+(12x1.008)+(6x16.00)=180.16
Amount of glucose (10.0 g)/(180.16 g mol^{-1}) = 0.0555 mol

Question: What mass of $FeSO_4.7H_2O$ do you need to dose an anaemic cat with 50 mg of iron?

Molar mass of Fe = 55.85
Amount of iron required is (0.050 g) / (55.85 g mol^{-1}) = 8.95×10^{-4} mol
Amount of iron sulfate in dose = 8.95×10^{-4} mol
Molar mass of $FeSO_4.7H_2O$ = 278.0
Mass of iron sulfate in dose = $8.95 \times 10^{-4} \times 278.0$ = 0.25 g

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Calculations involving moles

e.g. How much ethanol do I obtain from the fermentation of 1.0 kg of glucose? n=m/M

	$C_6H_{12}O_6$ (aq) $\longrightarrow$	$2C_2H_5OH$(aq) + $2CO_2$(g)
Mass/g	1000	510
Molar mass/gmol^{-1}	180.16	46.07
Amount/mol	5.55	11.10

Question: What mass of CO_2 is produced from the animal metabolism of 1.0 kg of glucose?

	$C_6H_{12}O_6$(aq) + $6O_2$(g) $\longrightarrow$	$6CO_2$(g) + $6H_2O$(l)
Mass/g	1000	1500 (2 sig figs)
Molar mass/gmol^{-1}	180.16	44
Amount/mol	5.55	33.3

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Gases

It may not be convenient to measure the *mass* of a gas

Properties of Gases:

- are compressible
- exert pressure
- expand to fill the entire volume of the container
- diffuse rapidly
- density (ρ) is << than liquids or solids.

A gas consists of very small, widely separated particles in rapid motion.

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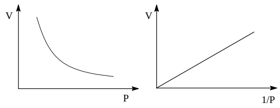
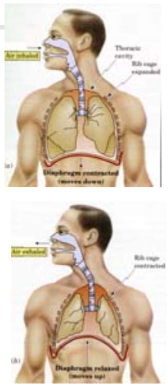
Gases

- Boyle noticed an inverse relationship between volume and pressure.

Pressure x volume = constant

PV = *a*



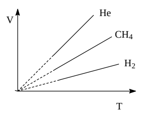


Gases

- Charles found the volume of a gas, at constant pressure, increased linearly with temperature.

Volume = constant x temperature

V = *b*T



Different gases extrapolated to zero volume at the same temperature. This is *absolute zero* at -273.15 °C = 0 K.

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Gases

- Avagadro proposed that equal volumes of gases at the same temperature and pressure contained the same number of "particles".

Volume = constant x No of moles

V = *c* n

$\left.\begin{array}{l} PV = a \\ V = bT \\ V = cn \end{array}\right\}$ **PV = nRT**

R = universal gas constant

= 8.3145 J mol^{-1} K^{-1}

= 0.082 L atm K^{-1} mol^{-1}

1 mole of any gas at standard temp & pressure (0 °C & 1 atm) occupies 22.4 L (or 24.4 L at 25 °C & 1 atm)

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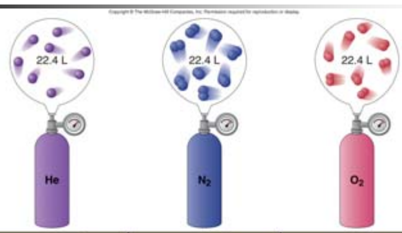
Gases



n = 1 mol	*n* = 1 mol	*n* = 1 mol
P = 1 atm (760 torr)	*P* = 1 atm (760 torr)	*P* = 1 atm (760 torr)
T = 0°C (273 K)	*T* = 0°C (273 K)	*T* = 0°C (273 K)
V = 22.4 L	*V* = 22.4 L	*V* = 22.4 L
Number of gas particles = 6.022×10^{23}	Number of gas particles = 6.022×10^{23}	Number of gas particles = 6.022×10^{23}
Mass = 4.003 g	Mass = 28.02 g	Mass = 32.00 g
d = 0.179 g/L	*d* = 1.25 g/L	*d* = 1.43 g/L

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Example

The mass of 1.00 L of a gas at 2.00 atm and 25 °C is 2.76 g. What is the molecular weight of the gas?

PV = nRT and n = m/M

(2.00 atm)(1.00 L) = n (0.082 L atm K^{-1} mol^{-1})(273 + 25 K)

∴ n = (2.00 / 24.436) mol = 0. 0 818 mol

M = 2.76 g / 0.0818 mol = 33.7 g mol^{-1} (H_2S)

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Question

What volume does 1500 g of CO_2 occupy at 1.0 atm and 38 ^{0}C?

$PV = nRT$ and $n = m/M$

Use $R = 0.082$ L atm K^{-1} mol^{-1} and $n = 1500$ g / 44 g mol^{-1} = 34 mol

(1.0 atm)(V) = (34 mol) (0.082 L atm K^{-1} mol^{-1})(273 + 38 K)

$\therefore$ V = (34 x 0.082 x 311 / 1.0) (mol L atm K^{-1} mol^{-1} K / atm)

= 867 L ~ 870 L

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Question – Air bags

Textbook: $2NaN_3(s) \rightarrow 2Na(s) + 3N_2(g)$!
$6NaN_3(s) + Fe_2O_3(s) \rightarrow 3Na_2O(s) + 2Fe(s) + 9N_2(g)$

How many grams of NaN_3 would be required to provide 75.0 L of nitrogen at 25 °C and 0.984 atm?

$PV = nRT$ and $n = m/M$ and $R = 0.082$ L atm K^{-1} mol^{-1}

Amount of nitrogen n = 0.984 x 75.0/0.0821 x 298 = 3.02 mol

Amount of NaN_3 required = 3.02 x 2/3 = 2.01 mol

Mass of NaN_3 required = mole x molar mass
= 2.01 x 65.0 = 131 g

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Partial pressures

In a mixture of gases, the total pressure exerted is the sum of the *partial pressures* that each gas would exert if it were alone.

$$P_{TOTAL} = p_A + p_B + p_C + ...$$

The partial pressure is related to the number of moles present, expressed as a mole fraction, x

Mole fraction of A = x_A = (No of moles of A) / (Total No of moles present)

Thus $p_A = x_A P_{TOTAL}$ and $p_B = x_B P_{TOTAL}$

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Partial pressures - example

Air consists of approximately 20 % oxygen and 80 % nitrogen. What are the partial pressures of these gases at 1 atm and 10 atm ?

Mole fraction of O_2 = x_{O2} = (20 %) / (20 % + 80 %) = 0.20
Mole fraction of N_2 = x_{N2} = (80 %) / (80 % + 20 %) = 0.80
(check: Σ mole fractions = 1)

At 1 atmosphere: p_{O2} = 0.20 x 1 atm = 0.2 atm
p_{N2} = 0.80 x 1 atm = 0.8 atm
(check: Σ partial pressure = total pressure)

At 10 atmosphere: p_{O2} = 0.20 x 10 atm = 2 atm
p_{N2} = 0.80 x 10 atm = 8 atm
(check: Σ partial pressure = total pressure)

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Significance $p = x P_{TOTAL}$

During a surgical procedure an animal may be ventilated to ensure a regular supply of oxygen to the brain. If the absorption of oxygen by the lungs is impaired it is desirable to increase the partial pressure of oxygen in the lungs.

This may be achieved by
- Increasing the total pressure
- Increase the mole fraction of O_2

Convenient to do surgery at atmospheric pressure

Breathing pure oxygen increases p_{O2} in the lungs by five times

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