# Lecture 1 - 5th September 2024

density: $\rho = \frac{m}{V}$ → water density: $997\ kg/m^3$

## Significant Digits

- all nonzero digits are significant!
- for quantities less than one, any zero preceding the first non-zero digit is not significant.
  - ↳ eg: 0.00237 has 3 sig figs.
- in quantities greater than one, any zero following the last non-zero digit is not significant, unless there is a decimal point.
  - ↳ eg: 200 has only one sig fig, while 200.00 has five.

- when adding or subtracting, retain digits to the magnitude of the value with the least significant digits.

- when multiplying or dividing, keep the same number of digits as the value with the least significant digits.

## Stoichiometry:

Example: what is $7.2\ \frac{Btu}{lbm\,°F}$ expressed in units of $J g^{-1} K^{-1}$?

↳ given: $1 J = 9.4782 \cdot 10^{-4}$ Btu, $1 kg = 2.20462$ lbm, $1 K = 1.8°F$

$$\hookrightarrow 7.2\ \frac{Btu}{lbm\,°F} \cdot \frac{1\ J}{9.4782 \cdot 10^{-4}\ Btu} \cdot \frac{2.20462\ lbm}{1\ kg} \cdot \frac{1 kg}{1000 g} \cdot \frac{1.8°F}{1 K}$$

$= 30.1 \frac{J}{gK}$

Example: you are interested in calculating the annual reduction in $CO_2$ emissions by replacing your car with an all-electric vehicle. Assume that you drive an annual distance 14000km. Your car has a fuel effeciency 28 miles per gallon. The electric car has an average energy consumption of 157 Wh/km.

↳ Data for $CO_2$ emission: 25g $CO_2$/kWh, 2.3 kg $CO_2$/L

↳ Gas: $$14000 \frac{km}{year} \cdot \frac{6.21371 \cdot 10^{-4} mi}{1 m} \cdot \frac{1000 m}{1 km} \cdot \frac{1 gal}{28 mi} \cdot \frac{1000 L}{264.172 gal} \cdot \frac{2.3 kg\, CO_2}{1 L} = 2705 \frac{kg\, CO_2}{year}$$

Electric: $$14000 \frac{km}{year} \cdot \frac{157 Wh}{1 km} \cdot \frac{25 g\, CO_2}{1 kWh} \cdot \frac{1 kWh}{1000 Wh} \cdot \frac{1 kg}{1000 g} = 55 \frac{kg\, CO_2}{year}$$

reductions: gas - electric = $2705 - 55 = 2650 \frac{kg\, CO_2}{year}$

## Temperature Conversions:

- $T(°F) = 1.8\, T(°C) + 32$
- $T(°C) = \frac{T(°F) - 32}{1.8}$
- $T(K) = T(°C) + 273.15$
- $T(°R) = 1.8\, T(K)$
- $T(°R) = T(°F) + 491.67$

all given on exams!

# Classification of Matter

All Matter
- seperatable → substance
  - decomposable → compound
  - not decomposable → element
- not seperatable → mixture
  - uniform → homogeneous
  - not uniform → heterogeneous

## Example: classify the following:

a) a piece of metal: can't determine

b) distilled water: pure substance

c) distilled water w/ ice: pure substance ↳ bc when seperated, both are still $H_2O$!

d) oil on water: heterogeneous

e) coffe w/ cream and sugar: heterogenous

| H |
|---|
| 1 → atomic number: # of protons |
| 1.00794 → relative atomic mass (u) |

↳ # protons + # electrons = relative atomic mass!

## Example: the mass number and the atomic number of an atom that contains 15 electrons, 15 protons, and 16 neutrons are, respectively:

15 protons means that the atomic number is 15.
the mass is # protons + # electrons = 15 + 16 = 31.

∴, 31 and 15.

- Atoms are most stable when their outer shell is completely empty or completely full.
  ↳ octet rule!

- Elements combine to form compounds by atomic bonding.

- Bonding involves electrons that are either shared (covalent bond) or transferred (ionic bond)

- Energy is absorbed or released when electrons are transferred or shared.

Example: copper has two major naturally occuring isotopes, which have 34 and 36 neutrons. Using the periodic table, determine the percentage abundance of copper atoms having 34 neutrons.

- From the periodic table, the atomic number of copper is 29 and the atomic mass is 63.546 amu.

↳ mass of $^{63}Cu$ : $29 + 34 = 63u$
  mass of $^{65}Cu$ : $29 + 36 = 65u$.

$$63.546u = x \cdot 63u + (1-x) \cdot 65u$$

$$\therefore, x = 0.727 = 72.7\%.$$

- Electronegativity: a measure of how strongly an atom competes for electrons in bonds formed with other atoms.
  ↳ increases rightwards in the periodic table!

Ionic Compounds: one atom donates one or more electron to another atom.
- Usually a metal combined with a non-metal.
- Dissociate into ions when dissolved in water.
  ↳ Eg: NaCl, ordered crystal of $Na^+$ and $Cl^-$ ions.

Covalent Compounds: one or more atoms share one or more electrons.
- Large, organic molecules are usually covalent.
- Do not dissociate into ions when dissolved in water.
  ↳ Eg: $CH_4$, $C_6H_{12}O_6$

- Two or more atoms, joined by covalent bonds, may form a charged polyatomic ion.
  ↳ Eg: ammonium ($NH_4^+$), carbonate ($CO_3^{2-}$), etc.

- Molecular formula: shows the actual number of atoms in a molecule.

- Emperical formula: gives the relative number of atoms in a molecule.

- The molecular formula can be obtained from the empirical formula if the molecular mass of the compound is known.

Example: $C_6H_{12}$ is the molecular formula, while $CH_2$ is the emperical formula of hexene.

Example: A compound has the empirical formula $CH_2O$ and a molecular weight of 150.13 u. What is the molecular formula?

↳ weight of C : 12.011
weight of $H_2$ : $1.008 \cdot 2 = 2.016$
weight of O : 15.999

∴, weight of $CH_2O = 12.011 + 2.016 + 15.999$
$= 30.026$ u.

we know that the compound should have a molecular mass of 150.13u, so how many times does one $CH_2O$ go into it?

$150.13 \div 30.026 = 5.$

∴, compound is $5CH_2O = C_5H_{10}O_5$.

• During a chemical reaction, atoms rearrange through the breaking and formation of chemical bonds.

- Chemical equations describe changes that occur in chemical reactions.
  - ↳ equations must be balanced (atom conversion principle)

## Balancing a chemical equation:

- Done by including stoichiometric coefficients
- The stoichiometric chemical equation describes only the net changes taking place in a reaction.

**Example:** $FeS + O_2 \longrightarrow Fe_2O_3 + SO_2$

- $2FeS + O_2 \longrightarrow Fe_2O_3 + SO_2$ — 2Fe, 2S, 2O → 2Fe, S, 5O
- ↳ $2FeS + O_2 \longrightarrow Fe_2O_3 + 2SO_2$ — 2Fe, 2S, 2O → 2Fe, 2S, 7O
- ↳ $4FeS + O_2 \longrightarrow 2Fe_2O_3 + 4SO_2$ — 4Fe, 4S, 2O → 4Fe, 4S, 14O
- ↳ $\underset{4Fe\ 4S}{4FeS} + \underset{14O}{7O_2} \longrightarrow \underset{4Fe}{2Fe_2O_3} + 4SO_2$ (14O)

**Example:** $NH_3 + O_2 \longrightarrow NO + H_2O$

- $2NH_3 + O_2 \longrightarrow 2NO + 3H_2O$ — 2N, 6H, 2O → 2N, 6H, 5O
- $2NH_3 + 4O_2 \rightarrow 2NO + 6H_2O$ — 2N, 6H, 8O → 2N, 12H, 8O
- $4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$ — 4N, 12H, 10O → 4N, 12H, 10O

**Example:** $Na_2CO_3 + Mg(NO_3)_2 \rightarrow MgCO_3 + NaNO_3$

↳ $Na_2CO_3 + Mg(NO_3)_2 \rightarrow MgCO_3 + 2NaNO_3$

**The mechanism equation:** describes the steps required to go from reactants to products at a molecular level.

**Sequential Reactions:** when the product of an initial chemical reactions becomes a reactant for further reactions.

↳ eg: $A + B \rightarrow C + D$
$C + E \rightarrow F$

$$\left.\begin{array}{l} A + B \rightarrow C + D \\ C + E \rightarrow F \end{array}\right\} A + B + E \rightarrow D + F$$

Example: consider a natural gas composed of a mixture of methane ($CH_4$) and ethane ($C_2H_6$) combusted in oxygen to form carbon dioxide and water. Write balanced chemical equations to describe what occurs.

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$
$$C_2H_6 + \frac{7}{2}O_2 \rightarrow 2CO_2 + 3H_2O$$

↳ since these are simultoneous reactions, we cannot add them.

• Never combine simultaneous reactions into a single equation!!

**Avogadro's Constant:** $6.022 \cdot 10^{23}$ units = 1 mole

↳ Example: 1 mole of $O_2$ molecules = $6.022 \cdot 10^{23}$ $O_2$ molecules
1 mole of apples = $6.022 \cdot 10^{23}$ apples

↳ 1 molecule of $CH_4$ contains 1 C atom and 4 H atoms, while 1 mol of $CH_4$ contains 1 mol of C and 4 mols of H.

- **Molar Mass/Weight:** the mass of one mole of a substance. ⟶ $M = \frac{m}{n}$

↳ Example: determine the molar mass of the following:

C: 12.011 g/mol
H: 1.0079 g/mol
O: 15.999 g/mol

these are just the mass given on the periodic table!!!

$C_7H_{14}O_2$: $7(12.011) + 14(1.0079) + 2(15.999)$
$= 130.186$ g/mol

- Since one mole of carbon is defined as 12g of $^{12}C$, the mass given on the periodic table is the molar mass!

Example: isopentyl acetate ($C_7H_{14}O_2$) is the compound responsible for the scent of bananas. Interestingly, bees release about 1μg of this compound when they sting to attract other bees to join the attack.

a) how many molecules of isopentyl acetate are released in a typical bee sting?

from previous example!

molar mass of $C_7H_{14}O_2$ = 130.186 g/mol

$\hookrightarrow 130.186 \dfrac{g}{mol} \cdot \dfrac{1 \ mol}{6.022 \cdot 10^{23} \ molecules} \cdot \dfrac{1 \ \mu g}{10^{-6} \ g}$

$= 2.1618 \cdot 10^{-16} \dfrac{\mu g}{molecule}$.

$\therefore, \dfrac{1}{2.1618 \cdot 10^{-16} \dfrac{\mu g}{molecule}} = 4.6 \cdot 10^{15} \dfrac{molecules}{\mu g}$

b) how many atoms of carbon are present in this?

$\hookrightarrow$ since each molecule of $C_7H_{14}O_2$ contains seven carbon atoms, $4.6 \cdot 10^{15}$ molecules of $C_7H_{14}O_2$ contain $7(4.6 \cdot 10^{15})$ carbon atoms.

$\therefore$, $3.2 \cdot 10^{16}$ Carbon atoms.

Example: the hemoglobin content of blood is about 15.5 g/100mL. The molar mass of hemoglobin is about 64500 g/mol. There are 4 iron atoms in a hemoglobin molecule. Approximately how many grams of iron are present in the 5 L of blood of a typical adult?

$5 \ L \ \cancel{blood} \times \dfrac{1000 \ \cancel{mL}}{1 \ \cancel{L \ blood}} \times \dfrac{15.5 \ \cancel{g \ hemoglobin}}{100 \ \cancel{mL \ blood}} \times \dfrac{1 \ \cancel{mol \ hemoglobin}}{64500 \ \cancel{g \ hemoglobin}}$

$\times \dfrac{4 \ \cancel{mol \ Fe}}{1 \ \cancel{mol \ hemoglobin}} \times \dfrac{55.845 \ g \ Fe}{1 \ \cancel{mol \ Fe}} = 2.7 g \ Fe$

Example: how many mols of $NaClO_3$ are needed to produce 6 mol of $SO_2$ in the following two-step reaction: $2NaClO_3 \rightarrow 2NaCl + 3O_2$

$S + O_2 \rightarrow SO_2$

Since $O_2$ is produced in the first reaction and used in the second, and since we aren't told that the equations happen simutaneously, we know that it's sequential.

↳ $2NaClO_3 \rightarrow 2NaCl + 3O_2$

$3S + 3O_2 \rightarrow 3SO_2$.

↳ $2NaClO_3 + 3S \rightarrow 2NaCl + 3SO_2$

to get 6 mols of $SO_2$, we simply multiply both sides of the reaction by 2:

$4NaClO_3 + 6S \rightarrow 4NaCl + 6SO_2$.

∴, 4 mols of $NaClO_3$ are needed to make 6 mols of $SO_2$.

Example: an approach for carbon capture is to dissolve carbon dioxide from power plant exhaust in water and then inject that solution into sub-surface basalt rocks that contain the mineral $Mg_2SiO_4$. The disssolved carbon dioxide will react with basalt to form the stable mineral, $MgCO_3$, according to the following unbalanced equation: $Mg_2SiO_4 + CO_2 \rightarrow SiO_2 + MgCO_3$.

a) What mass of $CO_2$, in g, can be stored in one tonne of $Mg_2SiO_4$?

First, we must balance the equation:

$$Mg_2SiO_4 + 2CO_2 \rightarrow SiO_4 + MgCO_3 .$$

$$1 \text{ tonne } Mg_2SiO_4 \times \frac{1000 \text{ kg}}{1 \text{ tonne}} \times \frac{1000 \text{ g}}{1 \text{ kg}} \times \frac{1 \text{ mol } Mg_2SiO_4}{140.69 \text{ g}} \times \frac{2 \text{ mol } CO_2}{1 \text{ mol } Mg_2SiO_4}$$

$$\times \frac{44.01 \text{ g } CO_2}{1 \text{ mol } CO_2} = 6.26 \cdot 10^5 \text{ g } CO_2 .$$

b) What mass of $MgCO_3$, in g, is produced?

$$1 \text{ tonne} \times \frac{1000 \text{ kg}}{1 \text{ tonne}} \times \frac{1000 \text{ g}}{1 \text{ kg}} \times \frac{1 \text{ mol } Mg_2SiO_4}{140.69 \text{ g}} \times \frac{2 \text{ mol } MgCO_3}{1 \text{ mol } Mg_2SiO_4} \times \frac{84.3139 \text{ g } MgCO_3}{1 \text{ mol } MgCO_3}$$

$$= 1.2 \cdot 10^6 \text{ g } MgCO_3 .$$

c) The average annual $CO_2$ emission per person is 17.7 tonne. What mass of $Mg_2SiO_4$, in tonne, is required to store Canada's annual $CO_2$ emission? Assume that the population of Canada is ~40 million.

$$17.7 \frac{\text{tonne}}{\text{person}} \times \frac{40{,}000{,}000 \text{ person}}{\text{population}} \times \frac{1 \text{ tonne } MgSiO_4}{6.26 \cdot 10^5 \text{ g } CO_2} \times \frac{10^6 \text{ g}}{1 \text{ tonne}}$$

$$= 1.13 \cdot 10^9 \frac{\text{tonne } Mg_2SiO_4}{\text{population}} .$$

Example: A natural gas is composed of 70 mol-% methane ($CH_4$) and 30 mol-% ethane ($C_2H_6$).

a) what is the average molar mass of the gas mixture?

$$1 \text{ mol} \times \frac{70 \text{ mol } CH_4}{100 \text{ mol}} \times \frac{(12.011)+4(1.008) \text{ g } CH_4}{1 \text{ mol } CH_4} = 11.23 \text{ g of } CH_4$$

$$1 \text{ mol} \times \frac{30 \text{ mol } C_2H_6}{100 \text{ mol}} \times \frac{2(12.011)+6(1.008)}{1 \text{ mol } C_2H_6} = 9.02 \text{ g of } C_2H_6$$

$\therefore$ total = $11.23 + 9.02 = 20.3$ g!

Example: how many grams of $CO_2$ are produced in the complete combustion of 406 g of a bottled gas that consists of 72.7 % $C_3H_8$ and 27.3% $C_4H_{10}$?

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$$

$$C_4H_{10} + 6.5\, O_2 \rightarrow 4CO_2 + 5H_2O$$

mass of $C_3H_8$: $406 \text{ g} \times \frac{72.7}{100} = 295.162 \text{ g } C_3H_8$

mass of $C_4H_{10}$: $406 \text{ g} - 295.162 \text{ g} = 110.838 \text{ g } C_4H_{10}$

$C_3H_8$: $3(12.011) + 8(1.008) = 44.09$ g/mol

$C_4H_{10}$: $4(12.011) + 10(1.008) = 58.12$ g/mol

we know $M = \frac{m}{n}$, so $n = \frac{m}{M}$:

$$n_{C_3H_8}: \frac{295.16 \text{ g}}{44.09 \text{ g/mol}} = 6.695 \text{ mol } C_3H_8$$

$$n_{C_4H_{10}}: \frac{110.838 \text{ g}}{58.12 \text{ g/mol}} = 1.907 \text{ mol } C_4H_{10}$$

from the reaction equations, we see that:

1 mol $C_3H_8$ ~ 3 mol $CO_2$, 1 mol $C_4H_{10}$ ~ 4 mol $CO_2$.

↳ mol $CO_2$ from $C_3H_8$ = 3(6.695) = 20.085 mol $CO_2$

mol $CO_2$ from $C_4H_{10}$ = 4(1.907) = 7.628 mol $CO_2$

∴ total mol $CO_2$ = 20.085 + 7.628 = 27.713 mol $CO_2$.

$$27.713 \text{ mol } CO_2 \times \frac{(12.011) + 2(16) \text{ g } CO_2}{1 \text{ mol } CO_2} = 27.713\ (44.011) \text{ mol } CO_2$$

= 1219.68 g $CO_2$ !

Example: a 10.2g sample of an organic compound containing carbon, hydrogen, and oxygen, was burned in excess oxygen. This yielded 23.1g $CO_2$ and 4.72g $H_2O$. Assuming complete combustion, what is the empirical formula of the compound?

- we know the C in the $CO_2$ and the H in the $H_2O$ must be from the original compound, but the O is both from the original compound and the excess oxygen.

$$23.1\text{g } CO_2 \times \frac{1 \text{ mol } CO_2}{44.009 \text{ g } CO_2} \times \frac{1 \text{ mol C}}{1 \text{ mol } CO_2} = 0.525 \text{ mol C}$$

$$4.72\text{g } H_2O \times \frac{1 \text{ mol } H_2O}{18.0148 \text{ g } H_2O} \times \frac{2 \text{ mol H}}{1 \text{ mol } H_2O} = 0.524 \text{ mol H}$$

$$0.525 \text{ mol C} \times \frac{12.011 \text{ g C}}{1 \text{ mol C}} = 6.3\text{g C}$$

$$0.524 \text{ mol } H \times \frac{1.008 \text{ g } H}{1 \text{ mol } H} = 0.528 \text{ g } H$$

$$m_O = m - m_C - m_H = 10.2 - 6.3 - 0.528 = 3.37 \text{ g } O$$

$$3.37 \text{ g } O \times \frac{1 \text{ mol } O}{16 \text{ g } O} = 0.211 \text{ mol } O$$

divide all by the smallest # of mols (0.211):

$$\frac{0.525}{0.211} \text{ mol } C, \quad \frac{0.524}{0.211} \text{ mol } H, \quad \frac{0.211}{0.211} \text{ mol } O$$

→ $C_{2.5}H_{2.5}O_1 = C_5H_5O_2$ !

**Solution**: composed of a solvent and one or more solutes.

- the solvent is present in the largest amount.
- for aqueous solutions (aq), the solvent is water.
- the solute is present in smaller amounts and is dissolved in the solvent
- solutions are homogeneous (have uniform properties).

**molarity**: describes the concentration of a solution.

→ $$\text{Molarity} = \frac{\text{amount of solute (moles)}}{\text{volume of solution (litres)}} \rightarrow C = \frac{n}{V}$$

**Example**: the fuel hydrazine can be produced by the reaction of solutions of sodium hypochlorite and ammonia:

$$NaClO_{(aq)} + 2NH_{3\,(aq)} \rightarrow N_2H_{4\,(aq)} + NaCl_{(aq)} + H_2O_{(l)}$$

a) 750 mL of a 0.8 M $NaClO$ solution is mixed with excess ammonia. How many moles of hydrazine can be formed?

we know $c = \frac{n}{V}$, so $n = c \cdot V$.

↳ $n = 0.8 \times 0.75 = 0.6$.

∴ 0.6 mol $N_2H_4$

b) If the final volume of the resulting solution is 1.25 L, what will be the molarity of the hydrazine?

↳ $c = \frac{n}{V} \rightarrow c = \frac{0.6}{1.25} = 0.48$ M.

· Other ways to express concentration:

- Percentages

↳ by mass: 25 % (w/w) = 25g solute per 100g solution

by volume: 25 % (v/v) = 25mL solute per 100mL solution

weight to volume: 25% (w/v) = 25g solute per 100mL solution

- molality = $\frac{\text{amount of solute (moles)}}{\text{amount of solvent (kg)}}$

- parts per million (ppm): $\frac{\text{g solute}}{\text{1,000,000 g solution}}$

- parts per billion (ppb): $\frac{\text{g solute}}{\text{1,000,000,000 g solution}}$

Example: an excess of aluminium foil is allowed to react with 225 mL of an aqueous solution of HCl that has a density of 1.088 g/mL and contains 18 % HCl by mass.

$$2\,Al_{(s)} + 6\,HCl_{(aq)} \rightarrow 2\,AlCl_{3\,(s)} + 3\,H_{2\,(g)}$$

What mass of $H_2$ is produced in the reaction?

mass = volume × density → mass = 0.225 mL × 1.088 $\frac{g}{mL}$
= 244.8 g.

18 % of this solution is HCl, so $0.18 \times 244.8\,g = 44.06\,g$ HCl

$$44.06\,g\ HCl \times \frac{1\ mol\ HCl}{36.46\,g\ HCl} \times \frac{3\ mol\ H_2}{6\ mol\ HCl} \times \frac{2.016\,g\ H_2}{1\ mol\ H_2} = 1.22\,g\ H_2$$

Example: a mixture contains only $CuCl_2$ and $FeCl_3$. A 0.7391 g sample of the mixture is completely dissolved in water and then treated with $AgNO_{3\,(aq)}$. The following reactions occur:

$$CuCl_{2\,(aq)} + 2\,AgNO_{3\,(aq)} \rightarrow 2\,AgCl_{(s)} + Cu(NO_3)_{2\,(aq)}$$
$$FeCl_{3\,(aq)} + 3\,AgNO_{3\,(aq)} \rightarrow 3\,AgCl_{(s)} + Fe(NO_3)_{3\,(aq)}$$

If it takes 86.91 mL of 0.1463 M $AgNO_3$ solution to precipitate all the chloride as AgCl, then what is the percentage by mass of copper in the original mixture?

we know that $m_{CuCl_2} + m_{FeCl_3} = 0.7391\,g$.

amount of $AgNO_3$ that reacts: $86.91\ mL \times \frac{1\,L}{1000\ mL} \times \frac{0.1463\ mol\ AgNO_3}{1\ L}$

$= 0.01271$ mol $AgNO_3$.

$\therefore, 0.01271 = n_{AgNO_3 \text{ in } 1} + n_{AgNO_3 \text{ in } 2}$

We see that 2 mol $AgNO_3$ ~ 1 mol $CuCl_2$

3 mol $AgNO_3$ ~ 1 mol $FeCl_3$

let $x$ be the moles of $CuCl_2$ and $y$ be the moles of $FeCl_3$.

↳ $0.01271 = 2x + 3y$

$0.7391 = m_{CuCl_2} + m_{FeCl_3} = n_{CuCl_2} M_{CuCl_2} + n_{FeCl_3} M_{FeCl_3}$

↓

$0.7391 = 134.452x + 162.204y$.

→ solve the system of equations: $x = 0.0019719$

$\therefore 0.0019719$ mol $CuCl_2$.

$$0.0019719 \text{ mol } CuCl_2 \times \frac{1 \text{ mol } Cu}{1 \text{ mol } CuCl_2} \times \frac{63.546 \text{ g } Cu}{1 \text{ mol } Cu} = 0.125 \text{ g } Cu.$$

↳ $\% \, Cu = \dfrac{0.125 \text{ g } Cu}{0.7391 \text{ g mixture}} = 16.95\%$ Cu by mass!

· Theoretical Yield: the expected yield from given quantities of reactants.

· Actual Yield: the quantity that is actually produced.

· Percentage Yield: the ratio of the actual yield to the theoretical yield

↳ $$\% \text{ yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100$$

Example: suppose that the reactions below occur consecutively, and each reaction has an 84% yield:

A: $CH_4 + Cl_2 \rightarrow CH_3Cl + HCl$

B: $CH_3Cl + Cl_2 \rightarrow CH_2Cl_2 + HCl$

Starting with 112g of $CH_4$ in reaction A and an excess of $Cl_2$, how many grams of $CH_2Cl_2$ are formed in reaction B?

$$112g\ CH_4 \times \frac{1\ mol\ CH_4}{16.04g\ CH_4} \times \frac{1\ mol\ CH_3Cl}{1\ mol\ CH_4} = 6.9825\ mol\ CH_3Cl$$

since we only have a 84% yield (not 100%):

$$6.9825 \times 0.84 = 5.86\ mol\ CH_3Cl$$

$$5.86\ mol\ CH_3Cl \times \frac{1\ mol\ CH_2Cl}{1\ mol\ CH_3Cl} \times \frac{84.93g\ CH_2Cl}{1\ mol\ CH_2Cl} = 497.6898.$$

however, we also only get 84% yield here as well:

$$0.84 \times 497.6898 = 418g\ CH_2Cl_2$$

- Limiting Reactant: the reactant that is completely consumed.
  - ↳ all other reactants are called excess reactants.

- Percentage excess is the proportion by which an excess reactant exceeds the stoichiometric amount.

- In stoichiometric calculations, we must use the limiting reactant as the basis!

Example: if 18.1 g of $NH_3$ is reacted with 90.4 g of CuO, what is the limiting reactant?

↳ $2NH_{3(g)} + 3CuO_{(s)} \rightarrow N_{2(g)} + 3Cu_{(s)} + 3H_2O_{(g)}$

molar mass of $NH_3$: $14.01 + 3(1.01) = 17.04$ g/mol

molar mass of CuO: $63.55 + 16 = 79.55$ g/mol

$$n = \frac{m}{M} \rightarrow \frac{18.1\text{ g}}{17.04\text{ g/mol}} = 1.062 \text{ mol } NH_3$$

$$\hookrightarrow \frac{90.4\text{ g}}{79.55\text{ g/mol}} = 1.137 \text{ mol CuO}$$

equation: 2 mol $NH_3$ ~ 3 mol CuO → $\frac{2 \text{ mol } NH_3}{3 \text{ mol CuO}} = 0.667$

actual: 1.067 mol $NH_3$ ~ 1.137 mol CuO → $\frac{1.067 \text{ mol } NH_3}{1.137 \text{ mol CuO}} = 0.937$

Since the actual mole ratio (0.937) is greater than the expected mole ratio (0.667), we have more $NH_3$ than needed.

↳ ∴, CuO is the limiting reactant!

Determine the theoretical yield of $N_2$ in grams.

$$90.4\text{ g CuO} \times \frac{1 \text{ mol CuO}}{79.545 \text{ g CuO}} \times \frac{1 \text{ mol } N_2}{3 \text{ mol CuO}} \times \frac{28.014 \text{ g } N_2}{1 \text{ mol } N_2}$$

$$= 10.612 \text{ g } N_2$$

- **Atom Economy** $= \dfrac{\text{mass of desired product(s)}}{\text{mass of all reactants}}$

↳ • calculated assuming a yield of 100 %.
  • based on the stoichiometry of the chemical equation and does not consider the mass of excess reactants.

## Postulates of Gas Behavior

1) a gas is composed of a very large number of molecules.
2) these molecules are seperated by a large distance relative to their own size.
3) these molecules are in ceaseless motion.

## Average Speeds:

1) most probable speed: $u_{mp} = \sqrt{\dfrac{2RT}{M}} = \sqrt{\dfrac{2k_BT}{m}}$

2) average speed: $u_{av} = \sqrt{\dfrac{8RT}{\pi M}} = \sqrt{\dfrac{8k_BT}{\pi m}}$

3) root-mean-squared speed: $u_{rms} = \sqrt{\dfrac{3RT}{M}} = \sqrt{\dfrac{3k_BT}{m}}$

where : $k_B = \dfrac{R}{N_A} = 1.3806 \times 10^{-23}\ J/K$

$R = 8.314\ J/(mol \cdot K)$

- higher temperature ⇒ broader range of speeds.

- distribution shifts towards higher speeds as temperature increases

- lower molecular weight $\Rightarrow$ broader range of speeds
- distribution shifts towards higher speeds for molecules with a lower molecular weight.

**Pressure:** $P = \frac{F}{A} = \frac{ma}{A}$ [Pa]

**Postulates of Gas Behavior (2):**

4) the molecules behave like hard spheres that undergo perfectly elastic collisions
5) there are no forces of attraction or repulsion

Kinetic-Molecular Theory (KMT)

↳ $PV = \frac{nMc^2}{3}$, where $c^2 = |v|^2$

- **Boyle's Law:** $P \propto \frac{1}{V}$, or $PV = a$

T must be in K!

- **Charles' Law:** $V \propto T$, or $V = bT$

- **Avogadro's Law:** the volume of a gas is proportional to the amount of gas. → $V \propto n$

↳ 0°C (273.15 K) and 1 atm: 1 mol gas = 22.414L

**The ideal gas law:** $PV = nRT$, where R is the gas constant. Most commonly, $R = 0.08206 \frac{atm \cdot L}{mol \cdot K}$

• note: $PV = nRT$ can also be expressed as $PV_m = RT$, where $V_m = \frac{V}{n}$ (the molar volume).

↳ any gas whose behavior conforms to the ideal gas law is called a perfect or an ideal gas. generally, it's a good approximation for many gasses at higher temperature and lower pressure.

• The temperature of an ideal gas is a measure of it's average translational kinetic energy.

• Gas Density: $\rho = \frac{PM}{RT}$

Example: a student accidentally swallows a drop of liquid oxygen, $O_{2(l)}$, which has a density of 1.149 g/mL. Assuming that the drop has a volume of 0.5 mL, what volume of gas will be produced at 37°C and 1 atm?

↳ $d = \frac{m}{V} \rightarrow m = V \cdot d = (1.149 \frac{g}{mL}) \times 0.5\ mL = 0.57\ g\ O_2$

ideal gas law: $PV = nRT = \frac{mRT}{M} \rightarrow V = \frac{mRT}{PM}$

mass, constant, temp (K), molar mass, pressure

$$V = \frac{(0.57)(0.08206)(37+273.15)}{(32)(1)} = 0.46\ L$$

Example: two bulbs of equal volume are connected by a tube of negligible volume. One of the bulbs has $T = 225\ K$, and the other has $T = 350\ K$. Exactly one mole of gas is injected into the system. Calculate the final number of moles of gas in each bulb.

we know that, at equilibrium, the pressure of the two bulbs is equal. Also, the 1 initial mole must be split between the two bulbs.

↳ ∴, $P_1 = P_2 = P$, and $n_1 + n_2 = 1$ mole

from the ideal gas law: $PV = nRT$

↳ $P_1 = \frac{n_1 R T_1}{V_1}$, and $P_2 = \frac{n_2 R T_2}{V_2}$.

since each bulb has equal volume, $V_1 = V_2 = V$.

∴, $P = P_1 = P_2 = \frac{n_1 R T_1}{V} = \frac{n_2 R T_2}{V} \longrightarrow n_1 T_1 = n_2 T_2$

from $n_1 + n_2 = 1$, we know $n_2 = 1 - n_1$.

∴, $n_1 T_1 = (1 - n_1) T_2 \rightarrow n_1 = \frac{T_2}{T_1 + T_2} = \frac{350}{225 + 350} = 0.61$ mol

∴, $n_1 = 0.61$ mol, $n_2 = 1 - n_1 = 0.39$ mol.

Example: NO can be produced according to the following balanced equation:

$6NaNO_{2(aq)} + 3H_2SO_{4(aq)} \rightarrow 4NO_{(g)} + 2HNO_{3(aq)} + 2H_2O_{(l)} + 3Na_2SO_{4(aq)}$

What volume (in L) of 0.646 M aqueous $NaNO_2$ should be used to produce 5L of NO at 20°C and at 0.97 atm?

how many moles of NO? → $PV = nRT \rightarrow n = \frac{PV}{RT}$

$\hookrightarrow n = \frac{(0.97)(5)}{(0.08206)(20 + 273.15)} = 0.2016$ mol NO

how many moles $NaNO_3$?

$\hookrightarrow 0.2016 \text{ mol NO} \times \frac{6 \text{ mol } NaNO_3}{4 \text{ mol NO}} = 0.3024 \text{ mol } NaNO_3$

$\rightarrow c = \frac{n}{V} \rightarrow V = \frac{n}{c} \rightarrow V = \frac{0.3024}{0.646} = 0.468 L$

Example: 3.57g of a potassium chloride - potassium chlorate ($KCl - KClO_3$) mixture decomposes by heat. 119 mL $O_2$ (g) is produced, measured at 22.4°C and 738 mmHg. What was the mass percent of $KClO_3$ originally?

$$2KClO_3 (s) \rightarrow 2KCl (s) + 3O_2 (g)$$

using $PV = nRT$, we can find the moles of $O_2$:

mmHg to atm!

$\hookrightarrow n_{O_2} = \frac{PV}{RT} = \frac{(\frac{738}{760})(119)}{(0.08206)(22.4 + 273.15)} = 0.0048 \text{ mol } O_2$

$0.0048 \text{ mol } O_2 \times \frac{2 \text{ mol } KClO_3}{3 \text{ mol } O_2} = 0.0032 \text{ mol } KClO_3$

molar mass of $KClO_3 = 39.1 + 35.45 + 3(16) = 122.55$ g/mol

↳ $m_{KClO_3} = M_{KClO_3} \times n_{KClO_3} \rightarrow m = 122.55 \frac{g}{mol} \times 0.0032\ mol$
$= 0.3922\ g\ KClO_3$.

mass percent: $\frac{\text{mass of solute}}{\text{total mass}} = \frac{0.3922}{3.57} \times 100 = 11\%$!

## • Dalton's Law of Partial Pressures

↳ what happens when two gasses are mixed?

↓

- different types of gasses in a mixture act independently of each other
- the total pressure of a mixture of a gas is the sum of the partial pressures of the components of the mixture → ie, $P = P_A + P_B + \ldots$

- Partial pressures are the pressures that each gas would have if present alone in a container of the same volume and at the same temp!

↳ $P_A = \frac{n_A RT}{V}$ and $P_B = \frac{n_B RT}{V}$ → assuming $V_A = V_B$

- $y_A = \frac{n_A}{n} = \frac{P_A V}{RT} \div \frac{PV}{RT} = \frac{P_A}{P}$ → gasses occupy same volume

- $y_A = \frac{n_A}{n} = \frac{PV_A}{RT} \div \frac{PV}{RT} = \frac{V_A}{V}$ → gasses under same pressure

↳ where $y_A$ is the mole fraction of gas A in the gas mixture!

**Example:** 2 g of He and 2g of $H_2$ are placed in a 15 L container at 30°C. What are their partial pressures, and what's the total pressure?

$$n = \frac{m}{M} \rightarrow n_{He} = \frac{2}{4.0026} = \frac{1}{2} \text{ mol He}$$

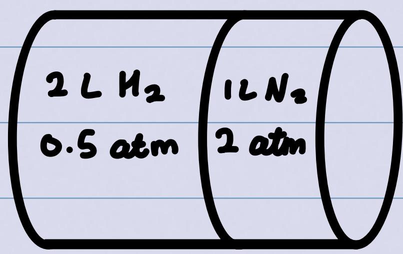
$$n_{H_2} = \frac{2}{2(1.008)} = 1 \text{ mol } H_2$$

$$P_{He} = \frac{n_{He}RT}{V} = \frac{(0.5)(0.08602)(30+273.15)}{15} = 0.829 \text{ atm}$$

$$P_{H_2} = \frac{n_{H_2}RT}{V} = \frac{(1)(0.08602)(30+273.15)}{15} = 1.65 \text{ atm}$$

$\therefore$, $P = P_{He} + P_{H_2} = 0.829 + 1.65 = 2.47$ atm

**Example:** what is the final total pressure if the barrier between the two containers is removed?




we know that $P_iV_i = P_fV_f$.

for $H_2$: $V_i = 2L$, $P_i = 0.5$ atm, $V_f = 3L$

$$\hookrightarrow P_{f_{H_2}} = \frac{P_iV_i}{V_f} = \frac{(0.5)(2)}{3} = \frac{1}{3} \text{ atm}$$

for $N_2$: $V_i = 1L$, $P_i = 2$ atm, $V_f = 3$ atm

$\hookrightarrow P_{f_{N_2}} = \frac{P_i V_i}{V_f} = \frac{(2)(1)}{3} = 2/3$ atm.

$\therefore, P = P_{f_{H_2}} + P_{f_{N_2}} = \frac{1}{3} + \frac{2}{3} = 1$ atm!

Example: a gaseous mixture of $C_2H_2$ and $CO$ is contained in a rigid vessel at 1.2 atm and 100 °C. The mixture is burned in an excess of $O_2$. The total pressure of the gaseous $CO_2$ and $H_2O$ produced by combustion was measured to be 2.88 atm in the same vessel at 100 °C.
What was the mole fraction of CO in the original $C_2H_2$ / CO mixture?

$C_2H_2 + O_2 \rightarrow CO_2 + H_2O$
$2C_2H_2 + 5O_2 \rightarrow 4CO_2 + 2H_2O$

$CO + O_2 \rightarrow CO_2$
$2CO + O_2 \rightarrow 2CO_2$

initial total pressure: $1.2 = P_{C_2H_2} + P_{O_2}$
final total pressure: $2.88 = P_{CO_2} + P_{H_2O}$

from the first reaction, we see that $n_{CO_2} = 2n_{C_2H_2}$
Since T and V remain constant, the mole ratios are equivalent to the partial pressure ratios
$\hookrightarrow P_{CO_2} = 2P_{C_2H_2}$ !

from the second reaction, $n_{CO_2} = n_{CO}$, so $P_{CO_2} = P_{CO}$

$P_{CO_2} = P_{CO_2,1} + P_{CO_2,2} = P_{CO}$
$P_{H_2O} = P_{C_2H_2}$

→ Solve the system of equations! → $P_{C_2H_2} = 0.84$ atm

$P_{CO} = 1.2 - 0.84 = 0.36$ atm.

$$y_{CO} = \frac{n_{CO}}{n_{mixture}} = \frac{P_{CO}}{P_{mixture}} = \frac{0.36}{1.2} = 0.3$$

• Intermolecular Forces:

↓

• Intermolecular Forces (IMFs) are forces of attraction between molecules.

• Not to be confused with intramolecular forces that hold atoms in a molecule together!

• many gasses behave as ideal gasses at high temperatures and low pressure <u>when IMFs do not play a large role!</u>

• London Dispersion Force

a) electrons are symmetrically distributed in a non-polar molecule

b) electrons may accumulate on one side of the molecule, creating an instantaneous dipole.

c) electrons in a neighboring molecule are now attracted to the positive side and perform an induced dipole.

- Polarizability: the tendency of charge distribution to become non-uniform in an atom or molecule
  ↳ what influences polarizability?
  ↓

- Dipole-Dipole Interactions: polar molecules have a permanent dipole moment (a positive end and a negative end)
  ↳ stronger than LDFs!

- Hydrogen Bonding:
  - highly electronegative atom pulls electrons away from H.
  - H is attracted to lone pair of electrons on a neighboring molecule
  - Occurs primarily between H and O, F, or N.
  - much stronger than van der Waals forces
  - much weaker than covalent bonds

- Repulsive Forces
  - arise due to electrostatic interactions as electron orbitals approach or overlap
  - very strong forces; important at short range

- Modifying the ideal gas law:
  ↳ we assumed that gas molecules have no volume. But, molecules do occupy space!

↳ $V = \frac{nRT}{P} + bn$, or $P = \frac{nRT}{V-bn}$

↳ we also assumed that there are no IMFs, but there are! ↗ esp at P↓, T↑ !

↳ Van der Waals' equation: $P = \frac{nRT}{V-nb} - \frac{an^2}{V^2}$

- Generally, higher temp ⇒ more ideal
  lower pressure ⇒ more ideal
  smaller atom / weaker IMFs ⇒ more ideal

Example: one mole of $SO_2$ occupies a volume of 1.85 L at 0°C and 10 atm. T or F?

a) $SO_2$ behaves like an ideal gas
↳ F → low T and high P

b) density of $SO_2$ is less than the density predicted by the ideal gas law
↳ $\frac{PM}{RT}$ → F

c) $SO_2$ molecules are attracting each other
↳ T

- Liquids

↳ molecules are free to move, but held close together by IMFs

↳ pressure of a liquid: $P = \rho g h$

pressure ↑ (P); density ↗ (ρ); g = 9.8 (g); ↳ height (h)