

Section 003

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Section 006

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C020-Fundamental Concepts

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The reverse calculations yield the formula of a compound from the % compositions given by experiment

Worked Example:

Calculate the molecular formula of a compound that is 58.77% C, 13.81% H, and 27.40% N, and whose molar mass = 204.4 g mol⁻¹

Assume 100 g of compound

$$\therefore \text{Mass of C} = 58.77 \text{ g}; n(\text{C}) = 58.77\text{g}/12.01 \text{ g mol}^{-1} = 4.893 \text{ mol}$$

$$\therefore \text{Mass of H} = 13.81 \text{ g}; n(\text{H}) = 13.81/1.008 = 13.70 \text{ mol}$$

$$\therefore \text{Mass of N} = 27.40 \text{ g}; n(\text{N}) = 27.40/14.01 = 1.956 \text{ mol}$$

Simplest molar ratio C: H: N = 4.893: 13.70: 1.956

$$= 2.502: 7.004: 1.000$$

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Making all the numbers into integers:
C:H: N = 5.004: 14.008: 2.000 ~ 5: 14: 2

∴ Empirical formula = $C_5H_{14}N_2$

Molar mass of the empirical formula = $5(12.0) + 14(1.01) + 2(14.0) \sim 102 \text{ g mol}^{-1}$

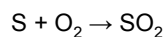
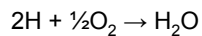
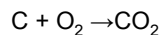
Since the molar mass of the sample = 204.4 g mol^{-1}

∴ Molecular formula = (empirical formula) x 2

∴ Molecular formula = $C_{10}H_{28}N_4$

Empirical Formulas by Experiment

The most common experimental method of obtaining empirical formulas is by **combustion analysis** where every element is converted to its most stable oxide on combustion



Except for N which is converted to N_2

For example: $C_5H_6NO_2 + O_2 \rightarrow CO_2 + H_2O + N_2$

Balanced: $C_5H_6NO_2 + (11/2)O_2 \rightarrow 5CO_2 + 3H_2O + \frac{1}{2}N_2$

By weighing the combustion products, one can determine the masses of the elements and the empirical formula of a compound

**** Worked Example:**

A 3.10 g sample of a compound containing C, H, and O only yielded 4.40 g CO₂ and 2.70 g of H₂O. What is the empirical formula?

Mass fraction of C in CO₂: $m(\text{C})/m(\text{CO}_2) = 12.0/44.0$

∴ mass C in compound = $(12.0/44.0) \times 4.40 \text{ g} = 1.20 \text{ g C}$

Mass fraction of H in H₂O = $2m(\text{H})/m(\text{H}_2\text{O}) = 2.02/18.0$

∴ mass of H in compound = $(2.02/18.0) \times 2.70 \text{ g} = 0.303 \text{ g H}$

The mass of O in compound can be obtained by the difference: $3.10 - 1.2 - 0.30 = 1.60 \text{ g}$

∴ in the unknown compound: # moles C = $1.20/12.0 = 0.1$

∴ $\text{C}_{0.1}\text{H}_{0.3}\text{O}_{0.1} = \text{CH}_3\text{O}$

mole H = $0.303/1.01 = 0.3$

moles O = $1.6/16.0 = 0.1$

Chemical Analysis

If a substance does **not** burn in oxygen, then the content of each element in a mixture can be determined by converting each element to a known compound whose mass can be measured

Worked Example:

A gold ring, known to be alloy of Cu and Au weighs 20.0 g.

If all the Cu is converted to 17.8 g CuCl₂ what is the % by mass of Au in the ring?

Mass fraction of Cu in CuCl₂ = $m(\text{Cu})/m(\text{CuCl}_2) = 63.5/136.5$

∴ mass of Cu in 17.8 g CuCl₂ = $(63.5/136.5) \times 17.8 \text{ g} = 8.28 \text{ g}$

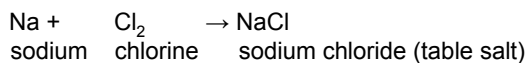
∴ mass of Au in the ring = $20.0 - 8.28 = 11.7 \text{ g}$

∴ % Au = $(11.7/20.0) \times 100\% = 58.5\%$ The ring is 14K gold

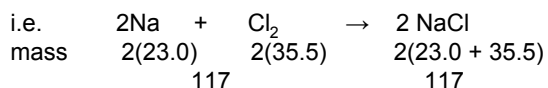
The Balanced Equation

A chemical equations indicates the **products** formed from **reactants**

For example:



The exact mass consequences of such a reaction can only be calculated if the **number of moles** of all reactants and products are equal



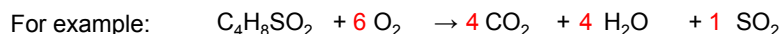
Calculations based on the mass relationship of **balanced** equations is termed **stoichiometry**

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Balancing simple chemical equations is simply a trial-and-error process of balancing individual atoms

- 1.) balance subscripts of highest subscripts first on the product side
- 2.) balance the rest of the atoms



**** Only balanced equations yield correct stoichiometric results**

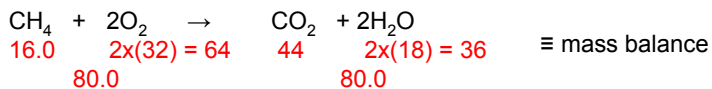
Mass relationships

A correctly balanced equation relates the # molecules, # moles, and the masses of products to reactants

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For example:
the combustion of natural gas, methane, CH₄



The numbers in red are the **ideal combining masses**, that is,
16.0 g CH₄ will react **completely** with 64.0 g of O₂ to yield 44.0 g CO₂ and 36.0 g H₂O

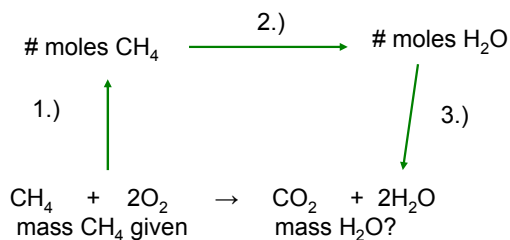
If the masses differ from ideal masses, one can calculate the extent of the reaction

Example:

if 34.0 g CH₄ is burned in an excess of O₂ what is the mass of H₂O produced?

There are **two** general ways of solving stoichiometry problems

i) The mole method



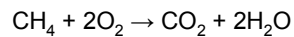
1.) # moles CH₄ present = 34.0/16.0 = 2.125 mol

2.) # moles H₂O present: $\frac{\text{CH}_4}{\text{H}_2\text{O}} \xrightarrow{\text{ideal ratio}} \frac{1}{2} \xrightarrow{\text{actual}} \frac{2.125}{x}$

x = 4.25 moles H₂O produced

3.) mass H₂O = 4.25 mol x 18.0 g mol⁻¹ = 76.5 g

ii) The direct mass method



Here we determine mass H_2O directly from the mass CH_4

$$\frac{\text{CH}_4}{\text{H}_2\text{O}} \xrightarrow{\text{ideal mass ratio}} \frac{16.0}{36.0} \xrightarrow{\text{actual}} \frac{34.0}{x}$$

$$x = 76.5 \text{ g}$$

The direct method is quicker for calculations requiring mass calculations, but the mole method is OK too (and it always works)
Both must be done **properly**

Limiting Reagent

Under most real conditions one reactant runs out before the other – termed the limiting reagent (L.R.)

The mass of the L. R. then determines the masses of all the species used/produced.

For example: 4 wagon frames + 12 wheels \rightarrow 3 wagons. L. R. \equiv wheels

Per Cent Yield

Under experimental conditions the mass of the product is usually less than the theoretical maximum.

The actual yield is expressed as:

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

Example:

In the combustion of 34.0 g CH₄ with 100 g O₂ a student collected 48.6 g H₂O. What is the percent yield of this experiment?

1.) Begin with a balanced equation:



3.) Determine which reactant is **limiting**

$$\text{ideal mass ratio} = \frac{\text{CH}_4}{\text{O}_2} = \frac{16.0}{64.0} = \frac{1}{4.0}$$

$$\text{actual mass ratio} = \frac{\text{CH}_4}{\text{O}_2} = \frac{34.0}{100.0} = \frac{1}{2.94}$$

Since $2.94 < 4.00$, O₂ is the L.R.

4.) Now calculate the maximum possible yield of H₂O based on O₂ as L. R.

$$\frac{\text{O}_2}{\text{H}_2\text{O}} = \frac{64.0}{36.0} = \frac{100}{x}$$

ideal actual

$$\rightarrow x = 56.3 \text{ g}$$

- 56.3 g H₂O is the maximum possible mass of H₂O that the conditions can yield

5.) Now calculate % yield:

$$\frac{\text{actual yield}}{\text{maximum yield}} = \frac{48.6}{56.3} \times 100\% = 86.3\%$$

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Reactions in Aqueous Solution

An aqueous solution of cations and anions will conduct electricity and is termed an **electrolyte**

The solubility of ionic compounds, in g per 100 mL, varies widely, but the following generalities are useful:

Very Soluble

Top Group I: Na⁺, K⁺, NH₄⁺ salts

Group VII: F⁻, Cl⁻, Br⁻, I⁻ salts

Strong acid anions: NO₃⁻, ClO₃⁻, SO₄²⁻

Poorly Soluble

Bottom Group II: Ca²⁺, Sr²⁺, Ba²⁺

Weak acid anions: CO₃²⁻, PO₄³⁻, C₂O₄²⁻,
CrO₄²⁻

Sulfides*: S²⁻

Oxides and hydroxides*: O²⁻, OH⁻

*Soluble if attached to Na⁺, K⁺, NH₄⁺ (Group I cations)

These soluble ions are often **spectator ions** in redox reactions (later)

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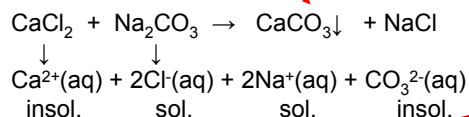
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Ionic Equations

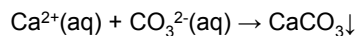
Often two ionic compounds will react with each other to produce a new ionic compound of low solubility.

This new compound will precipitate out of solution

Example:



The anions and cations that constitute the insoluble pair produce a net **ionic equation**:



The remaining soluble ions (Na^+ , Cl^-) are ignored as spectator ions

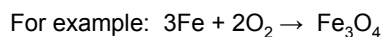
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Most Common Chemical Reactions

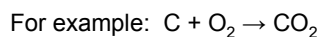
1.) Oxidation reactions (\equiv combustion)

Most elements react with O_2 to give stable oxides



They occur because the products are more stable than the reactants

Very exothermic reactions accompanied by heat/light (fire) = combustion



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Exchange Reactions

These proceed by the exchange of anion/cation pairs
- also know as **double replacement**

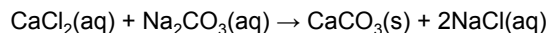
Commonly used to prepare desired compounds from more readily available ones

There are two major types:

a) Precipitation Reactions

In these the most soluble compounds form and precipitate from solution as in ionic equations

For example:

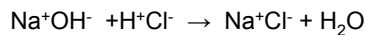


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b) acid-base reactions

For example:

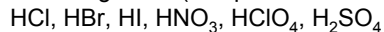


base acid salt water

In acid-base reactions, the **acid** supplies **H⁺** to a **proton acceptor**, the **base** (here OH⁻);
the remaining anion joins with the cation of the base to form a **salt**

Note:

There are 6 strong acids (complete dissociation):

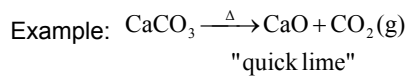


All others are weak acids (partial dissociation): much more later

c) Gas-forming Reactions

For example:

all metal carbonates



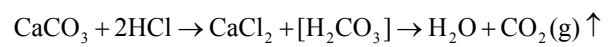
i) Lose CO₂ on heating (symbol = Δ)

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ii) React with acids

Example:



Gas evolution drives the reactions completely to the right; that is, they are not reversible