

**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<sup>-1</sup>

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 =  $5(12.0) + 14(1.01) + 2(14.0) \sim 102 \text{ g mol}^{-1}$

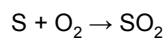
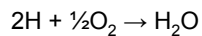
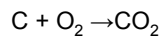
Since the molar mass of the sample =  $204.4 \text{ g mol}^{-1}$

∴ 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 CO<sub>2</sub> and 2.70 g of H<sub>2</sub>O. What is the empirical formula?

Mass fraction of C in CO<sub>2</sub>:  $m(\text{C})/m(\text{CO}_2) = 12.0/44.0$

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

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

∴ 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 CuCl<sub>2</sub> what is the % by mass of Au in the ring?

Mass fraction of Cu in CuCl<sub>2</sub> =  $m(\text{Cu})/m(\text{CuCl}_2) = 63.5/136.5$

∴ mass of Cu in 17.8 g CuCl<sub>2</sub> =  $(63.5/136.5) \times 17.8 \text{ g} = 8.28 \text{ g}$

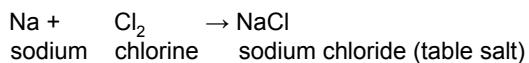
∴ mass of Au in the ring =  $20.0 - 8.28 = 11.7 \text{ g}$

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

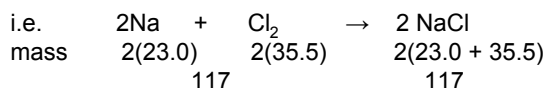
## The Balanced Equation

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



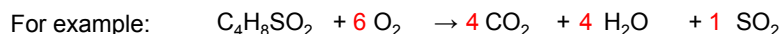
Calculations based on the mass relationship of **balanced** equations is termed **stoichiometry**

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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**

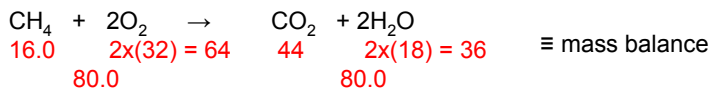
## Mass relationships

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, CH<sub>4</sub>



The numbers in red are the **ideal combining masses**, that is, 16.0 g CH<sub>4</sub> will react **completely** with 64.0 g of O<sub>2</sub> to yield 44.0 g CO<sub>2</sub> and 36.0 g H<sub>2</sub>O

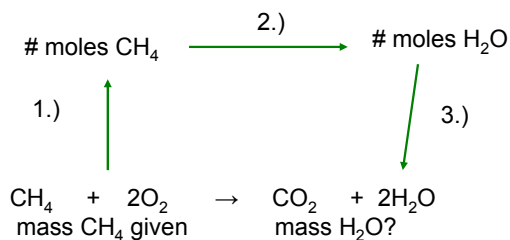
If the masses differ from ideal masses, one can calculate the extent of the reaction

**Example:**

if 34.0 g CH<sub>4</sub> is burned in an excess of O<sub>2</sub> what is the mass of H<sub>2</sub>O produced?

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

**i) The mole method**



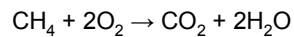
1.) # moles CH<sub>4</sub> present = 34.0/16.0 = 2.125 mol

2.) # moles H<sub>2</sub>O 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 H<sub>2</sub>O produced

3.) mass H<sub>2</sub>O = 4.25 mol x 18.0 g mol<sup>-1</sup> = 76.5 g

## ii) The direct mass method



Here we determine mass H<sub>2</sub>O directly from the mass CH<sub>4</sub>

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

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

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 → 3 wagons. L. R. ≡ 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 CH<sub>4</sub> with 100 g O<sub>2</sub> a student collected 48.6 g H<sub>2</sub>O. 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  $2.94 < 4.00$ , O<sub>2</sub> is the L.R.

4.) Now calculate the maximum possible yield of H<sub>2</sub>O based on O<sub>2</sub> 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 H<sub>2</sub>O is the maximum possible mass of H<sub>2</sub>O 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<sup>+</sup>, K<sup>+</sup>, NH<sub>4</sub><sup>+</sup> salts

Group VII: F<sup>-</sup>, Cl<sup>-</sup>, Br<sup>-</sup>, I<sup>-</sup> salts

Strong acid anions: NO<sub>3</sub><sup>-</sup>, ClO<sub>3</sub><sup>-</sup>, SO<sub>4</sub><sup>2-</sup>

### Poorly Soluble

Bottom Group II: Ca<sup>2+</sup>, Sr<sup>2+</sup>, Ba<sup>2+</sup>

Weak acid anions: CO<sub>3</sub><sup>2-</sup>, PO<sub>4</sub><sup>3-</sup>, C<sub>2</sub>O<sub>4</sub><sup>2-</sup>, CrO<sub>4</sub><sup>2-</sup>

Sulfides\*: S<sup>2-</sup>

Oxides and hydroxides\*: O<sup>2-</sup>, OH<sup>-</sup>

\*Soluble if attached to Na<sup>+</sup>, K<sup>+</sup>, NH<sub>4</sub><sup>+</sup> (Group I cations)

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

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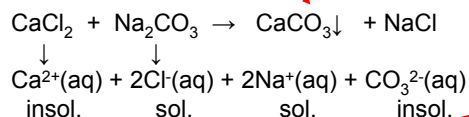


## Ionic Equations

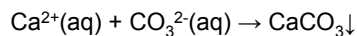
Often two ionic compounds will react with each other to produce a new ionic compound of low solubility.

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 ( $\text{Na}^+$ ,  $\text{Cl}^-$ ) are ignored as spectator ions

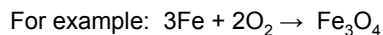
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## Most Common Chemical Reactions

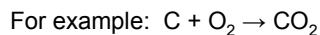
### 1.) Oxidation reactions ( $\equiv$ combustion)

Most elements react with  $\text{O}_2$  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**

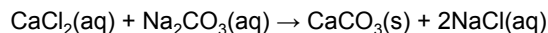
Commonly used to prepare desired compounds from more readily available ones

There are two major types:

### a) Precipitation Reactions

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

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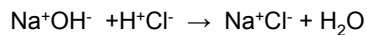


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### b) acid-base reactions

For example:

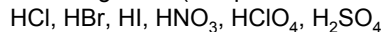


**base      acid      salt      water**

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

Note:

There are 6 strong acids (complete dissociation):

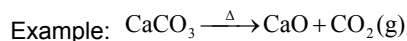


All others are weak acids (partial dissociation): much more later

### c) Gas-forming Reactions

For example:

**all** metal carbonates



i) Lose CO<sub>2</sub> on heating (symbol = Δ)

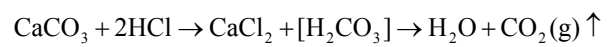
"quick lime"

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ii) React with acids

Example:



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