Quantitative aspects of chemical change
Grade 11 August 2020

Representing Chemical change

Balanced chemical equations

- Write and balance chemical equations. Use formulae for reactants and products and indicate the phases in brackets, i.e. (s), (ℓ), (g) and (aq).
- Interpret balanced reaction equations in terms of:
  - Conservation of atoms
  - Conservation of mass (use relative atomic masses)

Quantitative aspects of chemical change

The mole concept

- Describe the mole as the SI unit for amount of substance.
- Define one mole as the amount of substance having the same number of particles as there are atoms in 12 g carbon-12.
- Describe Avogadro's number, NA, as the number of particles (atoms, molecules, formula-units) present in one mole (NA = 6,023 x 10^{23} particles·mol^{-1}).
- Define molar mass as the mass of one mole of a substance measured in g·mol^{-1}.
- Calculate the molar mass of a substance given its formula.

Molar volume of gases

- State Avogadro's Law, i.e. one mole of any gas occupies the same volume at the same temperature and pressure.
- At STP: 1 mole of any gas occupies 22,4 dm^3 at 0 °C (273 K) and 1 atmosphere (101,3 kPa). Thus the molar gas volume, VM, at STP = 22,4 dm^3·mol^{-1}.

Volume relationships in gaseous reactions

- Interpret balanced equations in terms of volume relationships for gases, i.e. under the same conditions of temperature and pressure, equal amounts (in mole) of all gases occupy the same volume.

Concentration of solutions

- Define concentration as the amount of solute per litre of solution.
- Calculate concentration in mol·$ℓ^{-1}$ (or mol·dm^{-3}) using . $c = \frac{n}{v}$

More complex stoichiometric calculations

- Determine the empirical formula and molecular formula of compounds.
- Determine the percentage yield of a chemical reaction.
- Determine percentage purity or percentage composition, e.g. the percentage $CaCO^3$ in an impure sample of seashells.
- Perform stoichiometric calculations based on balanced equations that may include limiting reagents.

TABLE 3: THE PERIODIC TABLE OF ELEMENTS/*TABEL 3: DIE PERIODIEKE TABEL VAN ELEMENTE*

KEY/*SLEUTEL*: Atomic number / *Atoomgetal* (29); Electronegativity / *Elektronegatiwiteit* (1,9); Symbol / *Simbool* (Cu); Approximate relative atomic mass / *Benaderde relatiewe atoommassa* (63,5)

1 (I)	2 (II)	3	4	5	6	7	8	9	10	11	12	13 (III)	14 (IV)	15 (V)	16 (VI)	17 (VII)	18 (VIII)
1 2,1 H 1																	2 He 4
3 1,0 Li 7	4 1,5 Be 9											5 2,0 B 11	6 2,5 C 12	7 3,0 N 14	8 3,5 O 16	9 4,0 F 19	10 Ne 20
11 0,9 Na 23	12 1,2 Mg 24											13 1,5 Aℓ 27	14 1,8 Si 28	15 2,1 P 31	16 2,5 S 32	17 3,0 Cℓ 35,5	18 Ar 40
19 0,8 K 39	20 1,0 Ca 40	21 1,3 Sc 45	22 1,5 Ti 48	23 1,6 V 51	24 1,6 Cr 52	25 1,5 Mn 55	26 1,8 Fe 56	27 1,8 Co 59	28 1,8 Ni 59	29 1,9 Cu 63,5	30 1,6 Zn 65	31 1,6 Ga 70	32 1,8 Ge 73	33 2,0 As 75	34 2,4 Se 79	35 2,8 Br 80	36 Kr 84
37 0,8 Rb 86	38 1,0 Sr 88	39 1,2 Y 89	40 1,4 Zr 91	41 Nb 92	42 1,8 Mo 96	43 1,9 Tc	44 2,2 Ru 101	45 2,2 Rh 103	46 2,2 Pd 106	47 1,9 Ag 108	48 1,7 Cd 112	49 1,7 In 115	50 1,8 Sn 119	51 1,9 Sb 122	52 2,1 Te 128	53 2,5 I 127	54 Xe 131
55 0,7 Cs 133	56 0,9 Ba 137	57 La 139	72 1,6 Hf 179	73 Ta 181	74 W 184	75 Re 186	76 Os 190	77 Ir 192	78 Pt 195	79 Au 197	80 Hg 201	81 1,8 Tℓ 204	82 1,8 Pb 207	83 1,9 Bi 209	84 2,0 Po	85 2,5 At	86 Rn
87 0,7 Fr	88 0,9 Ra 226	89 Ac															

58 Ce 140	59 Pr 141	60 Nd 144	61 Pm	62 Sm 150	63 Eu 152	64 Gd 157	65 Tb 159	66 Dy 163	67 Ho 165	68 Er 167	69 Tm 169	70 Yb 173	71 Lu 175
90 Th 232	91 Pa	92 U 238	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

The Mole

Atoms, molecules and ions are too small to count, and there are so many particles in even the smallest sample of a substance.

There are more particles of water in a teaspoon then there are teaspoons of water in all the oceans.

Rather than dealing with the particles individually, we deal with a special number of particles.

The mole is a name for a special number. Many numbers have names, such as:

2 = pair

3 = hat-trick

12 = dozen

144 = gross

A mole of particles is an amount of $6,02 \times 10^{23}$ particles. $6,02 \times 10^{23}$ is known as Avogadro's number, N_A.

Avogadro's number (N_A) is too big to imagine. 602 000 000 000 000 000 000 000 .

This is many grains of sand, piled on the surface of the earth would almost reach the moon.

The **mole** is defined as the number of particles or atoms in 12,0 g of Carbon -12

Molar Mass

Particles are too small to weigh individually.

Molar mass (M) is defined as the mass of one mole of particles (atoms, molecules or formula units) and is measured in the unit g.mol^{-1}.

$$\text{number of mole (mol)} \longleftarrow n = \frac{m \rightarrow \text{mass of substance (g)}}{M \rightarrow \text{molar mass } (g \cdot mol^{-1})}$$

Relative atomic mass (Ar) is the average mass of an atom compared to the mass of a Carbon 12 atom. It is
measured in atomic mass units (amu).
Molar mass (M) of an element is equal to the magnitude of relative atomic mass (Ar) in *amu*. This is found on the periodic table. See the table below for other substances:

Type of substance	Particles	Example	Formula	Molar mass $g.mol^{-1}$
Element	Atoms	Neon	Ne	20
Covalent compound	Usually Molecules	Carbon dioxide	CO_2	12+32 = 44
Ionic compound	Ions (formula units)	Salt	NaCl	23+35,5 = 58,5
Metallic compound	Positive kernels and delocalized electrons	Gold	Au	197

Percentage Composition

$$\textbf{Percentage composition of element} = \frac{\textbf{molar mass of element}}{\textbf{M}_\textbf{R}\textbf{ of compound}} \times \textbf{100}$$

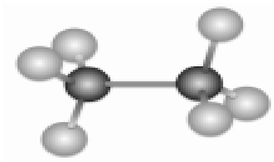
Consider these iron ores: haematite and magnetite – which contains more iron by mass?

Ore	Haematite	Magnetite
Formula	Fe_2O_3	Fe_3O_4
Relative molecular mass	(2 x 56) + (3 x 16) =160	(3 x 56) + (4 x 16) =232
% iron by mass	[(2 x 56) /160] x 100 = 70%	[(3 x 56) / 232] x 100 = 72%

∴ **magnetite contains more iron**

Different types of Chemical Formulae

Consider the substance ethane



Ball and stick model of ethane

It also can be represented using a formula. There are three types of formulas we use:

Molecular formula	Actual number of each atom.	Eg. C_2H_6
Empirical formula	Simplest whole number ratio of the atoms.	Eg.$C_1H_3 \rightarrow CH_3$
Structural formula	Shows how the atoms are joined.	H H H-C-C-H H H

EXAMPLE .1.
What is the relative formula mass of Calcium sulphate ($CaSO_4$)?
M_R ($CaSO_4$) = A_R (Ca) + A_R (S) + (4 x A_R (O))
= 40 + 32 + (4 x 16)
= 136 (no unit)

EXAMPLE. 2.

What is the molar mass of Calcium sulphate ($CaSO_4$)? =136 g.mol^{-1}

EXAMPLE. 3.

What is the relative molecular mass of sucrose ($C_{12}H_{22}O_{11}$)?

M_R ($C_{12}H_{22}O_{11}$) = 12 x A_R (C) + 22 x A_R (H)+ 11 x A_R (O)

= (12x 12) + (22x1) + (11 x 16)

= 342 (no unit)

EXAMPLE. 4.

What is the molar mass of sucrose($C_{12}H_{22}O_{11}$) ? = 342 g.mol

Concentrations of solutions

Solutions are homogeneous (uniform) mixtures of two or more substances. A solution is formed when a solute dissolves in a solvent.

The solvent and solute can be a gas, liquid, or solid. The most common solvent is liquid water. This is called an aqueous solution.

Solution	**Solute**	**Solvent**
Salt water	salt	water
Sugar water	sugar	water
Soda water	soda	water

Concentration

<u>Concentration is the amount of solute per litre of solution</u>.

The concentration of a solution is the number of mole of solute per unit volume of solution.

volume of solution.

number of moles (mol)

concentration (mol · dm^{-3}) ← $c = \frac{n}{V}$ → volume (dm^3)

can also be calculated with

$$c = \frac{m}{MV}$$

i.e. The number moles of solute per 1 dm³ of solution i.e. mol.dm^{-3}. If a solution of **potassium permanganate $KMnO_4$** has a concentration of 2 mol.dm^{-3} it means that for every 1 dm³ of solution, there are 2 moles of $KMnO_4$ dissolved in the solvent.

Note:
1000 cm³ = 1 dm³ (= 1 litre)
1 cm³ = 0,001 dm³
1 cm³ = 1 ml

EXAMPLE:

A solution contains 10 g of sodium hydroxide, NaOH, in 200 cm³ of solution. Calculate the concentration of the solution.

$$n(\text{NaOH}) = \frac{m}{M} = \frac{10}{23+16+1} = 0{,}25 \text{ mol}$$

$$V = 200 \text{ cm}^3 = 0{,}2 \text{ dm}^3$$

$$c(\text{NaOH}) = \frac{n}{V} = \frac{0{,}25}{0{,}2} = 1{,}25 \text{ mol} \cdot \text{dm}^{-3}$$

EXAMPLE:

Calculate the mass of solute in 600 cm³ of 1,5 mol·dm^{-3} sodium chloride solution.

$$V = 600 \text{ cm}^3 = 0{,}6 \text{ dm}^3$$

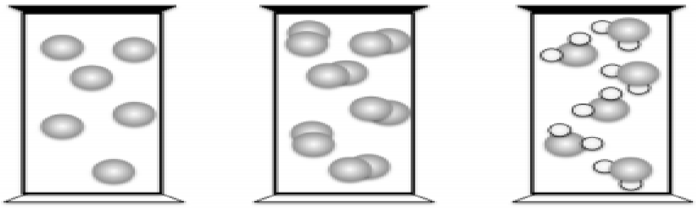
$$M(\text{NaCl}) = 23 + 35{,}5 = 58{,}5 \text{ g} \cdot \text{mol}^{-1}$$

$$n = cV = 1{,}5 \times 0{,}6 = 0{,}9 \text{ mol}$$

$$m = nM = 0{,}9 \times 58{,}5 = 52{,}65 \text{ g}$$

Molar Volumes of Gases

If different gases have the same volume under the same conditions of temperature and pressure, they will have the same number of molecules.



The molar volume of a gas, V_M, is the volume occupied by one mole of the gas.
V_M for all gases at STP is 22.4 $dm^3 \cdot mol^{-1}$.
Standard Temperature and Pressure (STP) is 273 K (0°C) and 1,01x10^5 Pa.
This also means that for reactions at constant temperature and pressure, gas volumes will react in the same ratio as the molar ratio.

molar ratio.

$$\begin{array}{ccccc} N_2 & + & 2O_2 & \rightarrow & 2NO_2 \\ 1\ \text{mol} & + & 2\ \text{mol} & \rightarrow & 2\ \text{mol} \\ 1\ \text{dm}^3 & + & 2\ \text{dm}^3 & \rightarrow & 2\ \text{dm}^3 \end{array}$$

$$\underset{\text{number of moles (mol)}}{n} = \frac{V \rightarrow \text{volume of gaseous substance } (dm^3)}{V_M \rightarrow \text{molar gas volume at STP } (22{,}4\ dm^3 \cdot mol^{-1})}$$

EXAMPLE:
A gas jar with a volume of 224 cm^3 is full of chlorine gas, at STP. How many moles of chlorine gas are there in the gas jar?

$n = V\frac{V}{V_M} = \frac{\mathbf{0.224}}{\mathbf{22.4}} = 0{,}01$ mol

Water of crystallization

Some ionic crystals trap a certain number of water molecules between the ions as they are forming. These water molecules are known as "Water of crystallization".

Eg. Hydrated copper sulphate:
$CuSO_4 \cdot \mathbf{5\ H_2O}$ has 5 water molecules per formula unit. When the hydrated salt crystals are heated, the water molecules evaporate off, leaving the anhydrous salt behind.

$CuSO_4 \cdot \mathbf{5\ H_2O(s)} \rightarrow CuSO_4\,(s) + \mathbf{5\ H_2O(g)}$

To calculate the number of moles of water of crystallization:

1. Calculate the mass of water that evaporated off.
2. Calculate the moles of water.
3. Calculate the moles of anhydrous salt.
4. Determine the ratio of water to anhydrous salt.
5. Write the formula for the hydrated salt.

Note:
The dot in the formula **(·)** between the salt and the water means that a light bond is formed. It is **NOT** a multiplication dot.

EXAMPLE:
13,2 g of a sample of zinc sulphate, $ZnSO_4.xH_2O$, was heated in a crucible. Calculate the number of moles of water of crystallisation if 7.4 g of solid remained.

1. $m(H_2O) = 13{,}2\ g - 7{,}4\ g$
$= 5{,}8\ g$

2. $n(H_2O) = \frac{m}{M} = \frac{5{,}8}{18} = 0{,}32$ mol

3. $n(ZnSO_4) = \frac{m}{M} = \frac{7{,}4}{161} = 0{,}046$ mol

4. ratio $= \frac{\text{mol water}}{\text{mol anhydrous salt}} = \frac{0{,}32}{0{,}046} = 1 : 7$

5. $\therefore$ formula $= ZnSO_4 \cdot 7H_2O$

Calculating the Empirical Formula from Percentage Composition

The empirical formula of a compound can also be found from its percentage composition. We assume that 100 g of the compound is analysed, then each percentage gives the mass of the element in grams in 100 g of the compound.

An **oxide of sulphur** contains 40% sulphur and 60% oxygen by mass. Determine the **empirical formula** of this oxide of sulphur.

Steps	Sulphur	Oxygen
Step 1: % of element	40	60
Step 2: Mass of element (g)	40	60
Step 3: Mol	n = m / M = 40 / 32 = 1,25 mol	n = m / M = 60 / 16 = 3,75 mol
Step 4: Smallest mol ratio	1,25 / 1,25 =1	3,75 /1,25 =3

Empirical formula: SO_3

Calculating the Empirical Formula of a Compound from Mass

Empirical formula is the chemical formula of a compound that shows the smallest whole number ratio of the atoms.

To calculate the empirical formula of a compound from mass:

1. Determine the mass of the elements.
2. Determine mol of each substance.
3. Simplify the atomic ratio.

EXAMPLE:
In a combustion reaction 0,48 g of magnesium ribbon is burnt. The amount of magnesium oxide produced is 0,80 g.
Calculate the **empirical formula** for **magnesium oxide**.

Steps	Magnesium	Oxygen
Step 1: Mass of element	0.48 g	0.80 – 0.48 = 0.32 g
Step 2: Mol (divide by mass of 1 mol)	n = m / M = 0.48 / 24 = 0,02 mol	n = m / M = 0.32 / 16 = 0,02 mol
Step 3: Atom ratio (divide by smallest no in ratio)	1	1

Empirical formula: MgO

EXAMPLE:
A sample of an **oxide of copper** contains 8 g of copper combined with 1 g of oxygen.
Find the **empirical formula** of the compound.

Steps	Copper	Oxygen
Step 1: Mass of element	8 g	1 g
Step 2: Mol (divide by mass of 1 mol)	n = m / M = 8 / 63,5 = 0,126 mol	n = m / M = 1 / 16 = 0,0625 mol
Step 3: Atom ratio (divide by smallest no in ratio)	0,126/0,0625 ≈2	0,0625/0,0625 =1

Empirical formula: Cu_2O

Empirical formula to Molecular Formula

The empirical formula is the simplest whole number ratio of atoms in a molecule. The molecular formula is the actual ratioof the atoms in a molecule.

The molecular formula can be calculated from the empirical formula and the relative molecular mass.

STEPS TO DETERMINE MOLECULAR FORMULA:

1. Determine the empirical formula (if not given).
2. Determine the molar mass of the empirical formula.
3. Determine the ratio between molecular formula and empirical formula.
4. Multiply the ratio into the empirical formula

EXAMPLE:

Butene has the empirical formula CH_2. The molecular mass of butene is 56g·mol^{-1}. Determine the molecular formula of butene.

1. Empirical formula given: CH_2
2. $M(CH_2) = 12 + 1 + 1$

$= 14\ g \cdot mol^{-1}$

3. ratio number = $\frac{molecular\ formula\ mass}{empirical\ formula\ mass}$

$= \frac{56}{14}$

$= 4$

4. $CH_2 \times 4 = C_4H_8$

Balanced chemical equations

Eg . $N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$

The balanced chemical equation is the "recipe". It tells us:

- The reactants used i.e. Nitrogen and Hydrogen
- The products produced. i.e. ammonia
- The states of the reactants and products (all gases here)
- The molar ratio of the reactants to products.

1 molecule of nitrogen reacts with 3 molecules of hydrogen to form 2 molecules of ammonia.

1 mole of nitrogen reacts with 3 moles of hydrogen to form 2 moles of ammonia.

Approach to reaction stoichiometry

1. Write a balanced chemical equation.
2. Change the 'given' amount into mole (use limiting reactant if applicable).
3. Determine the number of mole of the 'asked' substance using the mole ratio.
4. Determine the 'asked' amount from the number of mole

EXAMPLE:

To obtain iron, iron (III) oxide reacts with carbon monoxide according to the following word equation:

iron (III) oxide + carbon monoxide →iron + carbon dioxide

What mass of iron is produced from 48 g of iron (III) oxide?

1. $Fe_2O_3(s) + 3CO(g) \rightarrow 2Fe(s) + 3CO_2(g)$

2.

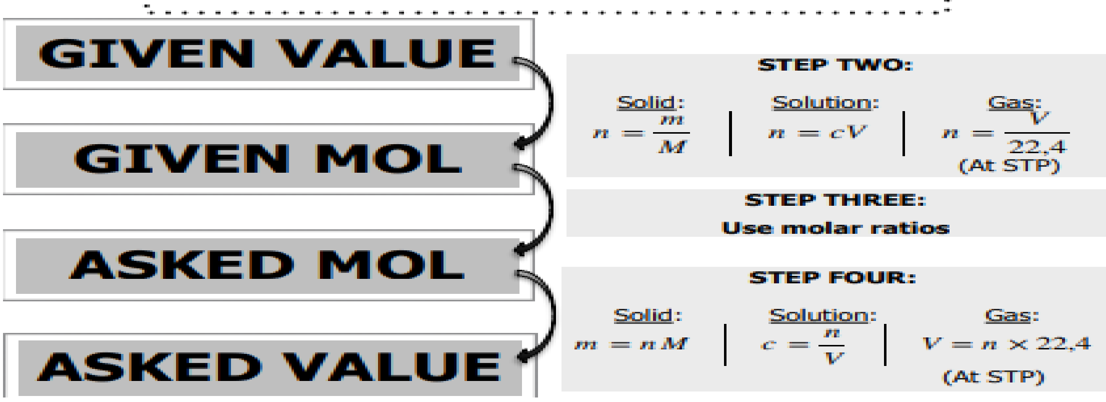
$$n(Fe_2O_3) = \frac{m}{M} = \frac{48}{160} = 0{,}3 \text{ mol}$$

3.

Fe_2O_3	:	Fe
1	:	2
0,3 mol	:	0,6 mol

4.

$$m(Fe) = nM = (0{,}6)(56) = 33{,}6 \text{ g}$$



Limiting Reactants

In a reaction between two substances, one reactant is likely to be used up completely before the other. This limits the amount of product formed.

Consider the reaction between magnesium and dilute sulphuric acid. The balanced chemical equation is $Mg(s) + H_2SO_4(aq) \rightarrow MgSO_4(aq) + H_2(g)$

This means that 1 mole of magnesium reacts with 1 mole of sulphuric acid. Both reactants will be completely used up by the time the reaction stops.

What happens if 1 mole of magnesium reacts with 2 mole of sulphuric acid? There is now insufficient magnesium to react with all of the sulphuric acid.

1 mole of sulphuric acid is left after the reaction.

All of the magnesium is used up, We say the magnesium is the limiting reactant. Some sulphuric acid is left after the reaction. We say the sulphuric acid is in excess.

The amount of limiting reactant will determine:

• The amount of product formed.

• The amount of other (excess) reactants used.

Determining limiting reactants

1. Calculate the number of moles of each reactant.
2. Determine the ratio between reactants.
3. Determine limiting reactant using the ratios.

NOTE:

If one reactant is in excess, it means that there is more than enough of it. If there are only 2 reactants and one is in excess, it means that the other is the limiting reactant

EXAMPLE:

A 8,4 g sample of nitrogen reacts with 1,5 g hydrogen. The balanced equation is:

$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$

Determine (a) which reactant is the limiting reactant, and (b) the mass of ammonia that can be produced.

(a)

1.

$$n(N_2) = \frac{m}{M} = \frac{8,4}{28} = 0,3 \text{ mol}$$

$$n(H_2) = \frac{m}{M} = \frac{1,5}{2} = 0,75 \text{ mol}$$

2.

N_2	:	H_2
1	:	3
0,3 mol	:	0,9 mol
0,25 mol	:	0,75 mol

Example 2

If all nitrogen is used, 0,9 mol hydrogen is needed, However, only 0,75 mol hydrogen is available. The hydrogen will run out first, therefore hydrogen is the limiting reactant.

(b)

Because the hydrogen is the limiting reactant, it will determine the mass of ammonia produced:

H_2	:	NH_3
3	:	2
0,75 mol	:	0,5 mol

$$m(NH_3) = nM = (0,5)(17) = 8,5 \text{ g}$$

Percentage Purity

Sometimes chemicals are not pure and one needs to calculate the percentage purity. Only the pure component of the substance will react. For an impure sample of a substance:

Percentage purity = $\frac{\textit{Mass of pure substance}}{\textit{Mass of impure substance}} \times 100$

STEPS TO DETERMINE THE PERCENTAGE PURITY

1. Determine moles of products.
2. From the balanced formula, determine the ratio between reactants and products.
3. Using the ratio, determine the number of moles of reactants.
4. Determine the mass of pure reactant.
5. Calculate the percentage purity of the sample

EXAMPLE:

An impure sample of calcium carbonate, $CaCO_3$, contains calcium sulphate, $CaSO_4$, as an impurity. When excess hydrochloric acid was added to 6g of the sample, 1200 cm^3 of gas was produced (measured at STP). Calculate the percentage purity of the calcium carbonate sample. The equation for the reaction is: $CaCO_3(s) + 2HCl(aq) \rightarrow CaCl_2(aq) + H_2O(l) + CO_2(g)$

1. $n(CO_2) = \frac{V}{V_M} = \frac{1,2}{22,4} = 0,054 \text{ mol}$

2.

$CaCO_3 : CO_2$

$1 : 1$

3.

$CaCO_3 : CO_2$

$1 : 1$

$0,054 : 0,054$

$\therefore$ 0,054mol $CaCO_3$ reacted

4.

$m(CaCO_3) = nM = (0,054)(40 + 12 + 16 + 16 + 16) = 5,4 \text{ g}$

5.

$\text{Percentage purity} = \frac{\text{Mass of pure substance}}{\text{Mass of impure substance}} \times 100$

$\text{Percentage purity} = \frac{5,4}{6,0} \times 100$

$\text{Percentage purity} = 90\ \%$

Percentage Yield

When you make a chemical in a laboratory a little of the chemical is always lost, due to evaporation into the surrounding air, or due to a little being left in solution.

Some of the reactants may not react. We say that the reaction has not run to completion.

This results in the amount of the chemical produced always being less than the maximum theoretical amount you would expect. We can express this by the percentage yield:

$\text{Percentage yield} = \frac{\text{Mass of product produced}}{\text{Maximum theoretical mass of product}} \times 100$

Percentage yield is usually determined using mass, but can also be determined with mol and volume.

STEPS TO DETERMINE THE PERCENTAGE YIELD

1. Determine moles of reactants.
2. From the balanced formula, determine the ratio between reactants and products.
3. Using the ratio, determine the number of moles of products.
4. Determine the theoretical mass of product.
5. Calculate the percentage yield.

EXAMPLE:

128g of sulphur dioxide, SO_2, was reacted with oxygen to produce sulphur trioxide, SO_3. The equation for the reaction is: $2SO_2(g) + O_2(g) \rightarrow 2SO_3(g)$

140g of SO_3 was produced in the reaction. Calculate the percentage yield of the reaction

1. $n(SO_2) = \frac{m}{M} = \frac{128}{64} = 2 \text{ mol}$

2.

$SO_2 : SO_3$

$2 : 2$

$1 : 1$

3.

$SO_2 : SO_3$

$1 : 1$

$2 : 2$

$\therefore$ 2 mol SO_3

4. $m(SO_3) = nM = (2)(32 + 16 + 16 + 16) = 160\text{g}$

5.

$\text{Percentage yield} = \frac{\text{Mass of product produced}}{\text{Maximum theoretical mass of product}} \times 100$

$\text{Percentage yield} = \frac{140}{160} \times 100$

$\text{Percentage yield} = 87.5\ \%$