Mass Relationships in Chemical Reactions

العلاقات الكتلية في التفاعلات الكيميائية

Atomic Mass

الكتلة الذرية

Atomic Mass

الكتلة الذرية

The mass of an atom depends on the number of electrons, protons and neutrons it contains.

تعتمد كتلة الذرة على عدد الإلكترونات و البروتونات و النيوترونات التي تحتويها

Atomic mass (sometimes called **atomic weight**): is the mass of the atom in atomic mass units (amu).

الكتلة الذرية (تسمى أحيانًا الوزن الذري): هي كتلة الذرة بوحدات الكتلة الذرية amu

Carbon-12 is the carbon isotope that has six protons and six neutrons. Setting the atomic mass of carbon-12 at 12 amu provides the standard for measuring the atomic mass of the other elements.

الكربون-12 هو نظير الكربون الذي يحتوي على ستة بروتونات وستة نيوترونات. ويُعدّ تحديد الكتلة الذرية للكربون-12 عند 12 وحدة كتل ذرية معيارًا لقياس الكتلة الذرية للعناصر الأخرى.

Avogadro's Number and Molar Mass of an Element

عدد أفوجادرو والكتلة المولية للعنصر

Mole

المول

Chemists measure atoms and molecules in **moles**.

يقيس الكيميائيون الذرات والجزيئات بالمولات.

In the SI system the **mole (mol)** is the amount of a substance that contains as many elementary entities (atoms, molecules, ions or other particles) as there are atoms in exactly 12 g of the carbon-12.

هو كمية المادة التي تحتوي على عدد من الكيانات الأولية (الذرات أو الجزيئات أو الأيونات أو الجسيمات الأخرى) يساوي عدد الذرات (mol في النظام الدولي للوحدات، المول) الموجودة في 12 غرامًا من الكربون-12.

The actual number of atoms in 12 g of carbon-12 is determined experimentally. This number is called Avogadro’s number (**N_A**), in honor of the **Amedeo Avogadro**.

يُحدد العدد الفعلي للذرات في 12 غرامًا من الكربون-12 تجريبيًا. ويُسمى هذا العدد عدد أفوجادرو تكريمًا لأميديو أفوجادرو.

The currently accepted value is:

$N_A = 6.0221415 \times 10^{23}$ **$\sim 6.022 \times 10^{23}$**

1 mole of hydrogen **atoms** contains 6.022 x 10^{23} H atoms.

1 mole of water **molecules** contains 6.022 x 10^{23} H_2O molecules.

1 mole of $SO4^{2-}$ **ions** contains 6.022 x 10^{23} $SO4^{2-}$ ions.

1 mole of **oranges** contains 6.022 x 10^{23} oranges.

1 mole of C-12 atoms has a mass of exactly 12 g and contains 6.022 x 10^{23} atoms.

This mass of C-12 is its **molar mass ($\mathcal{M}$),** defined as the mass (in grams) of 1 mole of units (such as atoms or molecules) of a substance.

The molar mass of C-12 (in grams) is numerically equal to its atomic mass in amu.

Likewise:

-the atomic mass of sodium (Na) is 22.99 amu and its molar mass is 22.99 g;
-the atomic mass of phosphorus (P) is 30.97 amu and its molar mass is 30.97 g; and so on.

Molar mass = (atomic mass of atom A x number of atom A) + (atomic mass of atom B x number of atom B) + ……

In calculations, the units of molar mass are g/ mol (SI unit).

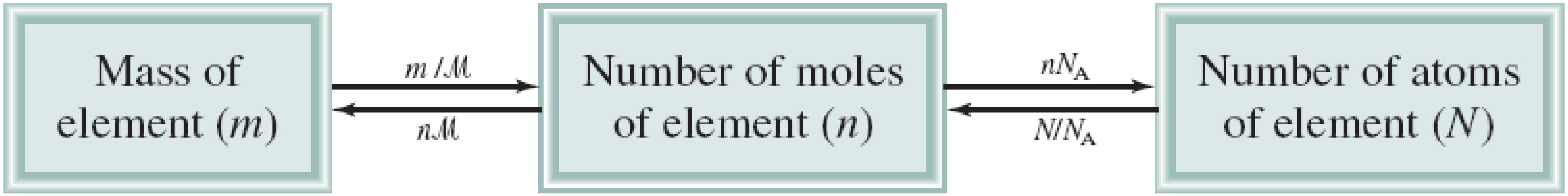
Example:

The molecular mass of $\mathbf{H_2O}$ is = 2 (atomic mass of H) + 1 (atomic mass of O)

= 2 (1.008) + (15.999) = 18.015 g / mol

The notions of Avogadro's number and molar mass enable us to carry out conversions between mass and moles of atoms and between moles and number of atoms

إن مفهومي عدد أفوجادرو والكتلة المولية يمكّناننا من إجراء التحويلات بين كتلة الذرات وعدد مولاتها، وبين عدد مولات الذرات وعددها.



Number of moles = Mass in gram / Molar mass

$$n = \frac{m}{\mathcal{M}}$$

Number of particles (ions, atoms, molecules,..etc) = Avogadro's no. x no. of moles

$$N = N_A \times n$$

N_A : Avogadro's no. = 6.022×10^{23} mol^{-1}

n : no. of moles

N : no. of atoms, molecules, ions or particles (unites)

$\mathcal{M}$: molar mass (g/mol)

m : mass (g)

EXAMPLE

Helium (He) is a valuable gas used in industry, low-temperature research, deep-sea diving tanks and balloons. How many moles of He atoms are in 6.46 g of He?

$$n = \frac{m}{\mathcal{M}} \Longrightarrow n = \frac{6.46\ \text{g}}{4\ \text{g/mol}} \Longrightarrow n = \mathbf{1.61\ mol\ of\ He}$$

EXAMPLE

Zinc (Zn) is a silvery metal that is used in making brass (with copper) and in plating iron to prevent corrosion. How many grams of Zn are in 0.356 mole of Zn?

$$n = \frac{m}{\mathcal{M}} \Longrightarrow m = n \times \mathcal{M} \Longrightarrow m = \mathbf{0.356\ mol \times 65.39\ g/mol}$$

$$\Longrightarrow m = \mathbf{23.3\ g\ of\ Zn}$$

EXAMPLE

Sulfur (S) is a nonmetallic element that is present in coal. When coal is burned, sulfur is converted to sulfur dioxide and eventually to sulfuric acid that gives rise to the acid rain phenomenon. How many atoms are in 16.3 g of S?

$$n = \frac{m}{\mathcal{M}} \Rightarrow n = \frac{16.3\ \text{g}}{32.07\ \text{g/mol}} \Rightarrow n = \mathbf{0.51\ mol\ of\ He}$$

$$N_A = \frac{N}{n} \Rightarrow N = n \times N_A \Rightarrow N = \mathbf{0.51\ mol \times 6.022 \times 10^{23}}$$

$$\Rightarrow N = \mathbf{3.06 \times 10^{23}\ S\ atoms}$$

EXAMPLE

How many hydrogen atoms are present in 25.6 g of urea [$(NH_2)_2CO$], which is used as a fertilizer, in animal feed, and in the manufacture of polymers? The molar mass of urea is 60.06 g/mol.

$$n = \frac{m}{\mathcal{M}} \Rightarrow n = \frac{25.6 \text{ g}}{60.06 \text{ g/mol}} \Rightarrow n = 0.43 \text{ mol of urea}$$

1 mol of urea ⇒ **4 mol of H**

0.43 mol of urea ⇒ **X mol of H**

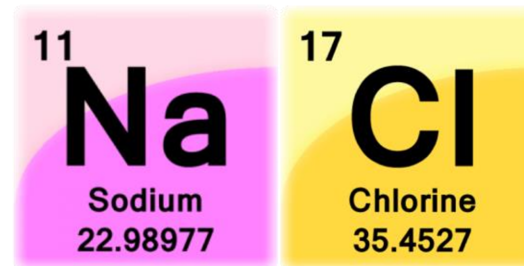
X mol of H = 1.7 mol

$$N = n \times N_A \Rightarrow N = 1.7 \text{ mol} \times 6.022 \times 10^{23} = 10.3 \times 10^{23} \text{ H atoms}$$

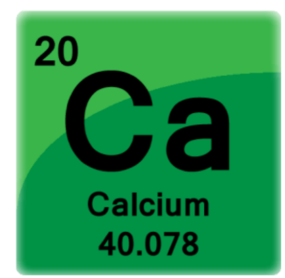
For ionic compounds like NaCl, MgO and $CaCl_2$ we use the term **formula mass**.

e.g., the formula unit of NaCl consists of one Na^+ ion and one Cl^- ion. Thus, the formula mass of NaCl is the mass of one formula unit: formula mass of NaCl = 22.99 + 35.45 = 58.44 g / mol

So its molar mass is 58.44 g / mol.



e.g., the formula mass of $CaCl_2$ = 40.08 + 2(35.45)
= 110.98 g / mol



Percent Composition of Compounds

التركيب النسبي للمركبات

The percent composition by mass is the percent by mass of each element in a compound.

التركيب المئوي بالكتلة هو النسبة المئوية بالكتلة لكل عنصر في المركب

Mathematically, the percent composition of an element in a compound is expressed as:

$$\text{percent composition of an element} = \frac{n \times \text{molar mass of element}}{\text{molar mass of compound}} \times 100\%$$

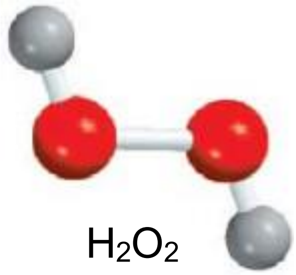
where *n* is the number of moles of the element in 1 mole of the compound.

e.g., in 1 mole of hydrogen peroxide (H_2O_2) there are 2 moles of H atoms and 2 moles of O atoms. The molar masses of H_2O_2, H, and O are 34.02 g, 1.008 g, and 16.00 g, respectively.

the percent composition of H_2O_2 is calculated as follows:

$$\%\text{H} = \frac{2 \times 1.008 \text{ g H}}{34.02 \text{ g H}_2\text{O}_2} \times 100\% = 5.926\%$$

$$\%\text{O} = \frac{2 \times 16.00 \text{ g O}}{34.02 \text{ g H}_2\text{O}_2} \times 100\% = 94.06\%$$

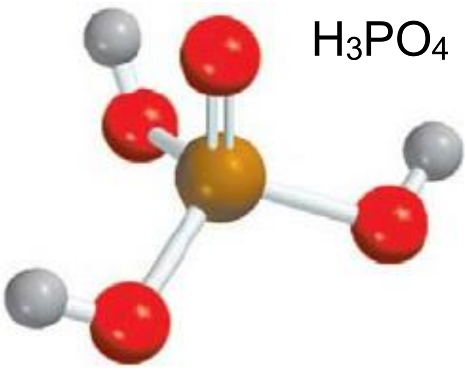


H_2O_2

The sum of the percentages is 5.926% + 94.06% = 99.99%. The small discrepancy from 100 percent is due to the way we rounded off the molar masses of the elements.

EXAMPLE

Phosphoric acid (H_3PO_4) is a colorless, syrupy liquid used in detergents, fertilizers, toothpastes, and in carbonated beverages for a “tangy” flavor. Calculate the percent composition by mass of H, P, and O in this compound.



The molar mass of H_3PO_4 = 97.99 g.

$$\%H = \frac{3(1.008\ g)\ H}{97.99\ g\ H_3PO_4} \times 100\% = 3.086\%$$

$$\%P = \frac{30.97\ g\ P}{97.99\ g\ H_3PO_4} \times 100\% = 31.61\%$$

$$\%O = \frac{4(16.00\ g)\ O}{97.99\ g\ H_3PO_4} \times 100\% = 65.31\%$$

The sum of the percentages is 3.086 + 31.61 + 65.31 = 100.01%.

EXAMPLE

Chalcopyrite ($CuFeS_2$) is a principal mineral of copper. Calculate the number of kilograms of **Cu** in 3.71×10^3 kg of chalcopyrite.

The molar masses of Cu and $CuFeS_2$ are 63.55 g and 183.5 g, respectively.
The mass percent of Cu is therefore

$$\%\text{Cu} = \frac{\text{molar mass of Cu}}{\text{molar mass of CuFeS}_2} \times 100\%$$
$$= \frac{63.55\text{ g}}{183.5\text{ g}} \times 100\% = 34.63\%$$

To calculate the mass of Cu in a 3.71×10^3 kg sample of $CuFeS_2$, we need to convert the percentage to a fraction (that is, convert 34.63 percent to 34.63/100, or 0.3463) and write

mass of Cu in $CuFeS_2$ = $0.3463 \times (3.71 \times 10^3 \text{ kg}) = 1.28 \times 10^3$ kg

Determination of Empirical Formulas

تحديد الصيغ التجريبية

Suppose that in one experiment the combustion of 11.5 g of ethanol produced 22.0 g of CO_2 and 13.5 g of H_2O. We can calculate the mass of C & H in ethanol sample as follows:

Firstly, calculate the number of mole for each atom: 1

mol of CO_2 $\longrightarrow$ 1 mol of C

22 g / 44 $\longrightarrow$ X then **mole of C = 0.5 mol**

1 mol of H_2O $\longrightarrow$ 2 mol of H

13.5 g / 18 $\longrightarrow$ X then **mole of H = 1.5 mol**

1 mol of C_2H_5OH $\longrightarrow$ 1 mol of O

11.5 g / 46 $\longrightarrow$ X then **mole of O = 0.25 mol**

Atom type	No. of moles	Ratio by divided on the smallest no. of moles	Ratio
C	0.5	0.5 / 0.25	2
H	1.5	1.5 / 0.25	6
O	0.25	0.25 / 0.25	1

The ratio of the atoms to each others is C : H : O as (2 : 6 : 1)

So, the empirical formula we obtained is **C_2H_6O**.

Molecular formula from empirical formula

الصيغة الجزيئية من الصيغة التجريبية

From percentage compositions we can obtain the empirical formula. We can obtain the molecular formula from the empirical formula if we are given the molecular weight.

يمكننا الحصول على الصيغة الأولية من خلال النسب المئوية للمكونات. ويمكننا الحصول على الصيغة الجزيئية من الصيغة الأولية إذا عُلم الوزن الجزيئي.

This whole number multiple is the ratio between the molecular and empirical formulas weight.

يمثل هذا العدد الصحيح النسبة بين وزن الصيغة الجزيئية ووزن الصيغة التجريبية.

$$\text{Whole-number multiple} = \frac{\text{molecular weight}}{\text{empirical formula weight}}$$

e.g.,

$$\frac{\mathcal{M}\ H_2O_2}{\mathcal{M}\ HO} = 2 \qquad \frac{\mathcal{M}\ C_6H_{12}O_6}{\mathcal{M}\ CH_2O} = 6$$

EXAMPLE

A sample of a compound contains 1.52 g of nitrogen (N) and 3.47 g of oxygen (O). The molar mass of this compound is 90 g. Determine the molecular formula and the accurate molar mass of the compound.

Atom type	No. of moles	Ratio by divided on the smallest no. of moles	Ratio
N	1.52 / 14 = 0.108	0.108 / 0.108	1
O	3.47 / 16 = 0.217	0.217 / 0.108	2

The ratio of the atoms to each others is N : O as (1 : 2)

So, the empirical formula we obtained is **NO_2**.

The empirical formula weight is equal to (1x 14) + (2x 16) = 46 g / mol.

$$\text{Whole-number multiple} = \frac{\text{molecular weight}}{\text{empirical formula weight}}$$

Whole-number multiple = 90 / 46 = 2

So, the molecular formula is: Whole-number multiple X EF = 2 (**NO_2**)

The MF is **N_2O_4**.

EXAMPLE

Ascorbic acid (vitamin C) cures scurvy. It is composed of 40.92 percent carbon (C), 4.58 percent hydrogen (H), and 54.50 percent oxygen (O) by mass. Determine its empirical formula.

Suppose;

we have 100 g of ascorbic acid, then each percentage can be converted directly to grams. In this sample, there will be 40.92 g of C, 4.58 g of H, and 54.50 g of O.

Atom type	No. of moles	Ratio by divided on the smallest no. of moles	Ratio
C	40.92 / 12 = 3.41	3.41 / 3.41	1
H	4.58 / 1 = 4.58	4.58 / 3.41	1.34
O	54.50 / 16 = 3.41	3.41 / 3.41	1

The ratio of the atoms to each others is C : H : O as (1 : 1.34 : 1)

The whole number of atoms must be as an integer, we cannot accept that there is 1.34 atoms of H, so we have to multiple **ALL** the ratio with the same number to get integers.

Because 1.34 x 3 gives us an integer 4, we multiply all the subscripts by 3 and obtain **$C_3H_4O_3$** as the empirical formula for ascorbic acid.

Chemical Reactions and Chemical Equations

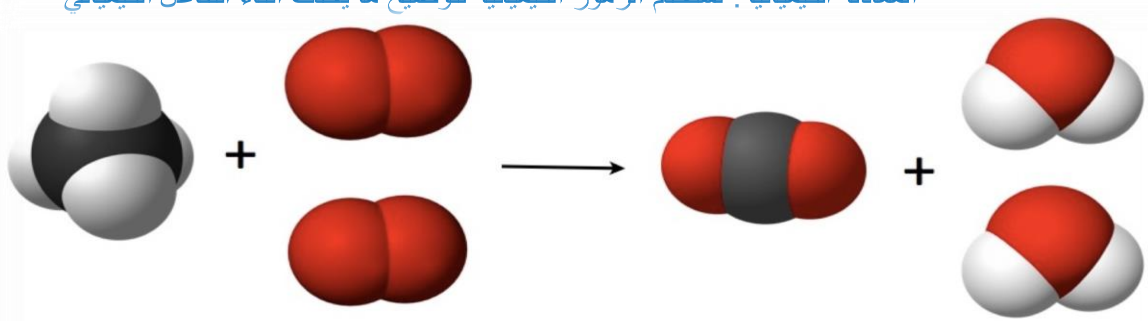
التفاعلات الكيميائية والمعادلات الكيميائية

A **chemical reaction**: a process in which a substance (or substances) is changed into one or more new substances.

التفاعل الكيميائي: عملية يتم فيها تحويل مادة (أو مواد) إلى مادة جديدة واحدة أو أكثر

A **chemical equation**: uses chemical symbols to show what happens during a chemical reaction.

المعادلة الكيميائية: تستخدم الرموز الكيميائية لتوضيح ما يحدث أثناء التفاعل الكيميائي



$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$

Writing Chemical Equations

كتابة المعادلات الكيميائية

What happens when hydrogen gas (H_2) burns in air (which contains oxygen, O_2) to form water (H_2O). This reaction can be represented by the chemical equation

$$H_2 + O_2 \longrightarrow H_2O$$

means "reacts with"
means "to yield"

This symbolic expression can be read: Molecular hydrogen reacts with molecular oxygen to yield water. The reaction is assumed to proceed from left to right as the arrow indicates.

To conform with the **law of conservation of mass**, there must be the same number of each type of atom on both sides of the arrow (we should balance the equation).

(balanced equation)

$$2H_2 + O_2 \longrightarrow 2H_2O$$

$2H_2$	$+ O_2$	$\longrightarrow 2H_2O$
Two molecules	+ one molecule	$\longrightarrow$ two molecules
2 moles	+ 1 mole	$\longrightarrow$ 2 moles

$$2H_2 + O_2 \longrightarrow 2H_2O$$

In the equation:

- H_2 and O_2 are the **reactants**, which are the starting materials in a chemical reaction.
- Water is the **product**, which is the substance formed as a result of a chemical reaction.

$$\text{reactants} \longrightarrow \text{products}$$

The **states** of the reactants and products are written in parentheses to the right of each compound; (*g*) gas, (*l*) liquid, (*s*) solid or (*aq*) aqueous solution.

Examples:

$$2CO(g) + O_2(g) \longrightarrow 2CO_2(g)$$

$$2HgO(s) \longrightarrow 2Hg(l) + O_2(g)$$

$$NaCl(s) \xrightarrow{H_2O} NaCl(aq)$$

$$CH_{4\,(g)} + 2\ O_{2\,(g)} \longrightarrow CO_{2\,(g)} + 2\ H_2O_{(g)}$$

Reactants appear on the left side of the equation.

تظهر المواد المتفاعلة على الجانب الأيسر من المعادلة

Products appear on the right side of the equation.

تظهر المنتجات على الجانب الأيمن من المعادلة

The **states** of the reactants and products are written in parentheses to the right of each compound; (*g*) gas, (*l*) liquid, (*s*) solid, (*aq*) aqueous solution.

تُكتب حالات المواد المتفاعلة والناتجة بين قوسين على يمين كل مركب؛ (g) غاز، (l) سائل، (s) صلب، (aq) محلول مائي

Subscripts present within a formula and tell the number of atoms of each element in a molecule.

تشير الأرقام السفلية الموجودة داخل الصيغة إلى عدد ذرات كل عنصر في الجزيء

Coefficients are inserted in front of a formula to balance the equation.

Sometimes the conditions (such as temperature or pressure) under which the reaction proceeds appear above or below the reaction arrow. Δ refer to temperature.

تُضاف المعاملات قبل الصيغة لتحقيق التوازن في المعادلة.

أحيانًا، تظهر الظروف (مثل درجة الحرارة أو الضغط) التي يحدث فيها التفاعل أعلى أو أسفل سهم التفاعل. يشير الرمز Δ إلى درجة الحرارة.

Balancing Chemical Equations

موازنة المعادلات الكيميائية

In the laboratory, small amounts of oxygen gas can be prepared by heating potassium chlorate ($KClO_3$). The products are oxygen gas (O_2) and potassium chloride (KCl). From this information, we write

$$KClO_3 \longrightarrow KCl + O_2$$

$$2KClO_3 \longrightarrow 2KCl + 3O_2$$

Check the number of each element

Reactants	Products
K (2)	K (2)
Cl (2)	Cl (2)
O (6)	O (6)

Heating potassium chlorate produces oxygen, which supports the combustion of wood splint.

EXAMPLE

The combustion (that is, burning) of the natural gas component ethane (C_2H_6) in oxygen or air, which yields carbon dioxide (CO_2) and water.

$$C_2H_6 + O_2 \longrightarrow CO_2 + H_2O$$

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

However, we normally prefer to express the coefficients as whole numbers rather than as fractions.

$$2C_2H_6 + 7O_2 \longrightarrow 4CO_2 + 6H_2O$$

EXAMPLE

When aluminum metal is exposed to air, a protective layer of aluminum oxide (Al_2O_3) forms on its surface.

$$Al + O_2 \longrightarrow Al_2O_3$$

$$2Al + \frac{3}{2}O_2 \longrightarrow Al_2O_3$$

However, equations are normally balanced with the smallest set of whole number coefficients.

$$4Al + 3O_2 \longrightarrow 2Al_2O_3$$

Amounts of Reactants and Products

كميات المواد المتفاعلة والنواتج

Stoichiometry

القياس الكمي

How much product will be formed from specific amounts of starting materials (reactants)?

ما مقدار المنتج الذي سيتكون من كميات محددة من المواد الأولية (المتفاعلات)؟

How much starting material must be used to obtain a specific amount of product?

ما مقدار المواد الأولية اللازمة للحصول على كمية محددة من المنتج؟

Stoichiometry is the quantitative study of reactants and products in a chemical reaction.

علم القياس الكمي هو الدراسة الكمية للمتفاعلات و النواتج في التفاعل الكيميائي.

To interpret a reaction quantitatively, we need to apply our knowledge of molar masses and the mole concept.

لتفسير التفاعل كمياً، نحتاج إلى تطبيق معرفتنا بالكتل المولية ومفهوم المول.

Mole method, which means that the stoichiometric coefficients in a chemical equation can be interpreted as the number of moles of each substance.

طريقة المول، والتي تعني أنه يمكن تفسير المعاملات القياسية في المعادلة الكيميائية على أنها عدد مولات كل مادة

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

The stoichiometric coefficients show that one molecule of N_2 reacts with three molecules of H_2 to form two molecules of NH_3. It follows that the relative numbers of moles are the same as the relative number of molecules:

$N_2(g)$	+	$3H_2(g)$	$\longrightarrow$	$2NH_3(g)$
1 molecule		3 molecules		2 molecules
1 mol		3 mol		2 mol

This equation can also be read as "1 mole of N_2 gas combines with 3 moles of H_2 gas to form 2 moles of NH_3 gas".

In stoichiometric calculations,

$$3 \text{ mol } H_2 \simeq 2 \text{ mol } NH_3$$
$$1 \text{ mol } N_2 \simeq 2 \text{ mol } NH_3$$
$$1 \text{ mol } N_2 \simeq 3 \text{ mol } H_2$$

the symbol $\simeq$ means "stoichiometrically equivalent to".

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

e.g., 6.0 moles of H_2 react completely with N_2 to form NH_3. Calculate the amount of NH_3 produced in moles?

<u>From balanced equation:</u>

3 mol of H_2 → 2 mol of NH_3

So, 6 mol of H_2 → X mol of NH_3

(6)(2) = 3X → X = **4 mol of NH$_3$ will be produced**.

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e.g., Suppose 16.0 g of H_2 react completely with N_2 to form NH_3. How many grams of NH_3 will be formed?

<u>From balanced equation:</u>

3 mol of H_2 → 2 mol of NH_3

So, (16 g / 2) mol of H_2 → X mol of NH_3

(16/2)(2) = 3X → X = **5.3 mol of NH$_3$ will be produced**.

Mass of NH_3 = (mol of NH_3)(molar mass of NH_3) = (5.3 mol)(17 g/mol) = **90.6 g of NH$_3$ will be formed.**

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

Similarly, we can calculate the mass in grams of N_2 consumed in this reaction.

<u>From balanced equation:</u>

3 mol of H_2 → 1 mol of N_2

So, (16 g / 2) mol of H_2 → X mol of N_2

(16/2)(1) = 3X → X = **2.6 mol of N_2 will be produced**.

Mass of N_2 = (mol of N_2)(molar mass of N_2) = (2.6 mol)(28 g/mol) = **74.6 g of N_2 will be formed.**

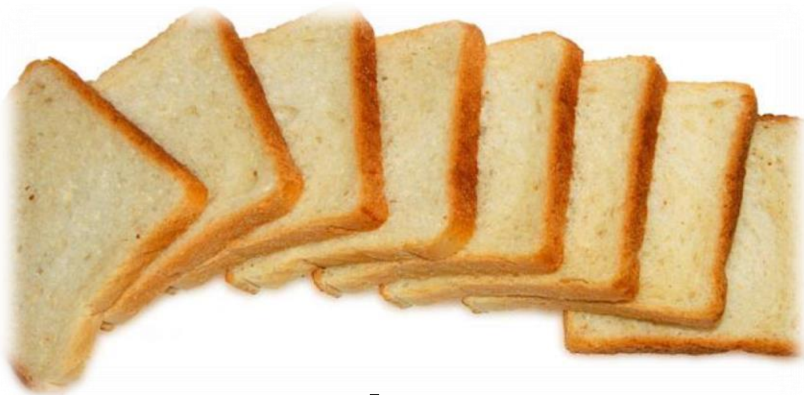
Limiting Reagents

الكواشف المحددة

Limiting Reagents

الكواشف المحددة

How Many Cheese Sandwiches Can I Make?



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→

The amount of available bread limits the number of sandwiches.

Limiting reagent (limiting reactant): the reactant used up first in a reaction, because the maximum amount of product formed depends on how much of this reactant was originally present. When this reactant is used up, no more product can be formed.

العامل المحدد (المتفاعل المحدد): هو المتفاعل الذي يُستهلك أولاً في التفاعل، لأن الحد الأقصى لكمية الناتج المتكون يعتمد على كمية هذا المتفاعل الموجودة أصلاً. عند استهلاك هذا المتفاعل، لا يمكن تكوين المزيد من الناتج.

Limiting reagent is completely consumed in a reaction (present in the smallest stoichiometric amount). Its called **limiting regent**; because it determines or limits the amount of product formed.

العامل المحدد هو العامل الذي يُستهلك بالكامل في التفاعل (يوجد بأقل كمية مكافئة). يُسمى العامل المحدد لأنه يُحدد أو يُقيد كمية الناتج المتكون.

Excess reagents are the reactants present in quantities greater than necessary to react with the quantity of the limiting reagent.

المواد المتفاعلة الزائدة هي المواد المتفاعلة الموجودة بكميات أكبر من اللازم للتفاعل مع كمية المادة المتفاعلة المحددة.

EXAMPLE

$$2\,H_2(g) + O_2(g) \longrightarrow 2\,H_2O(g) \qquad 2 \text{ mol } H_2 \simeq 1 \text{ mol } O_2$$

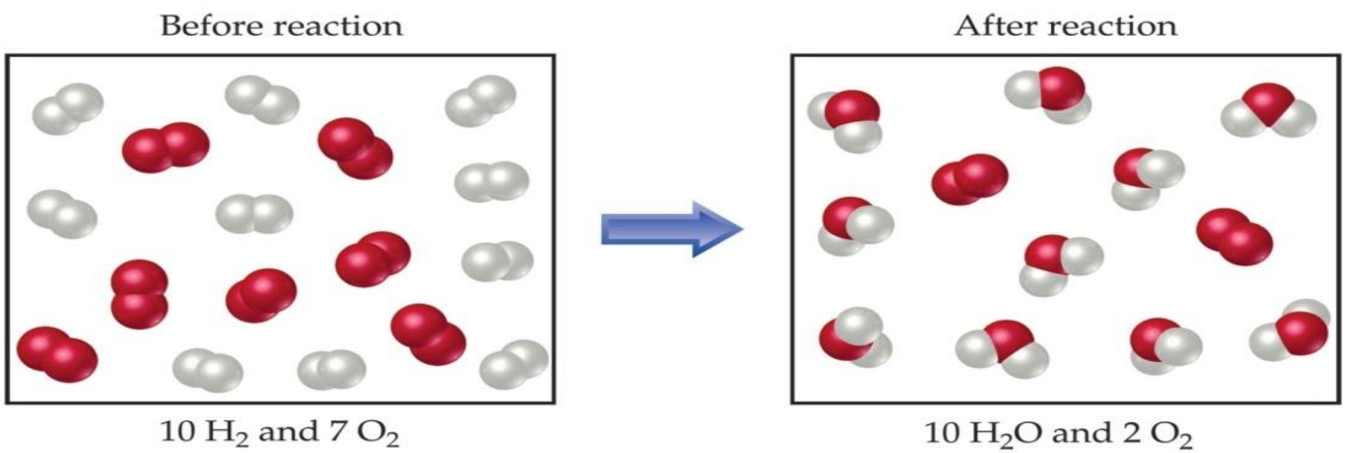
Suppose, mixture of 10 mole H_2 and 7 mole O_2 react to form water.

The number of O_2 needed to react with all the H_2 is:

2 mol of H_2 → 1 mol of O_2

So, 10 mol of H_2 → X mol of O_2

No. of mol of O_2 = 5 mol



In this example, H_2 would be the **limiting reactant**, which means that once all the H_2 has been consumed the reaction stops. And O_2 would be the **excess reactant**, and some is left over when the reaction stops.

EXAMPLE

Consider the industrial synthesis of methanol (CH_3OH) from carbon monoxide and hydrogen at high temperatures:

$$CO(g) + 2H_2(g) \longrightarrow CH_3OH(g)$$

Suppose initially we have 4 moles of CO and 6 moles of H_2.

In stoichiometric calculations involving limiting reagents, the first step is to decide which reactant is the limiting reagent.

One way to determine the limiting reagent is to calculate the number of moles of CH_3OH obtained based on the initial quantities of CO and H_2; the limiting reagent will yield the **smaller** amount of the product.

$$4\ \cancel{\text{mol CO}} \times \frac{1\ \text{mol CH}_3\text{OH}}{1\ \cancel{\text{mol CO}}} = 4\ \text{mol CH}_3\text{OH}$$

$$6\ \cancel{\text{mol H}_2} \times \frac{1\ \text{mol CH}_3\text{OH}}{2\ \cancel{\text{mol H}_2}} = 3\ \text{mol CH}_3\text{OH}$$

Because H_2 results in a smaller amount of CH_3OH, it must be the limiting reagent. Therefore, CO is the excess reagent.

EXAMPLE

Urea [$(NH_2)_2CO$] is prepared by reacting ammonia with carbon dioxide:

$$2NH_3(g) + CO_2(g) \longrightarrow (NH_2)_2CO(aq) + H_2O(l)$$

In one process, 637.2 g of NH_3 are treated with 1142 g of CO_2.
(a) Which of the two reactants is the limiting reagent?
(b) Calculate the mass of $(NH_2)_2CO$ formed.
(c) How much excess reagent (in grams) is left at the end of the reaction?

(a)
from NH_3

$$\text{moles of } (NH_2)_2CO = 637.2 \text{ g } \cancel{NH_3} \times \frac{1 \text{ mol } \cancel{NH_3}}{17.03 \text{ g } \cancel{NH_3}} \times \frac{1 \text{ mol } (NH_2)_2CO}{2 \text{ mol } \cancel{NH_3}} = 18.71 \text{ mol } (NH_2)_2CO$$

from CO_2

$$\text{moles of } (NH_2)_2CO = 1142 \text{ g } \cancel{CO_2} \times \frac{1 \text{ mol } \cancel{CO_2}}{44.01 \text{ g } \cancel{CO_2}} \times \frac{1 \text{ mol } (NH_2)_2CO}{1 \text{ mol } \cancel{CO_2}} = 25.95 \text{ mol } (NH_2)_2CO$$

NH_3 is the limiting reagent because it produces a smaller amount of $(NH_2)_2CO$.

(b) We determined the moles of $(NH_2)_2CO$ produced in part (a), using NH_3 as the limiting reagent. The molar mass of $(NH_2)_2CO$ is 60.06 g.

$$\text{mass of } (NH_2)_2CO = 18.71 \text{ mol } (NH_2)_2CO \times \frac{60.06 \text{ g } (NH_2)_2CO}{1 \text{ mol } (NH_2)_2CO}$$
$$= 1124 \text{ g } (NH_2)_2CO$$

(c) We can determine the amount of CO_2 that reacted to produce 18.71 moles of $(NH_2)_2CO$. The amount of CO_2 left over is the difference between the initial amount and the amount reacted.

Starting with 18.71 moles of $(NH_2)_2CO$, we can determine the mass of CO_2 that reacted

$$\text{mass of } CO_2 \text{ reacted} = 18.71 \text{ mol } (NH_2)_2CO \times \frac{1 \text{ mol } CO_2}{1 \text{ mol } (NH_2)_2CO} \times \frac{44.01 \text{ g } CO_2}{1 \text{ mol } CO_2}$$
$$= 823.4 \text{ g } CO_2$$

The amount of CO_2 remaining (in excess) is the difference between the initial amount and the amount reacted:

$$\text{mass of } CO_2 \text{ remaining} = 1142 \text{ g} - 823.4 \text{ g} = 319 \text{ g}$$

Reaction Yield

ناتج التفاعل

Theoretical yield of the reaction, is the amount of product that would result if all the limiting reagent reacted. The theoretical yield, then, is the maximum obtainable yield, predicted by the balanced equation.

الناتج النظري للتفاعل هو كمية الناتج التي ستتكون إذا تفاعل كل الكاشف المحدد. وبالتالي، فإن الناتج النظري هو أقصى ناتج يمكن الحصول عليه، والذي تتنبأ به المعادلة الكيميائية الموزونة.

Actual yield is the amount of product actually obtained (in practice) from a reaction, is almost always less than the theoretical yield.

إن العائد الفعلي هو كمية المنتج التي يتم الحصول عليها فعليًا (عمليًا) من التفاعل، وهو دائمًا تقريبًا أقل من العائد النظري.

To determine how efficient a given reaction is, chemists often figure the **percent yield**, which describes the proportion of the actual yield to the theoretical yield. It is calculated as follows:

لتحديد مدى كفاءة تفاعل معين، يحسب الكيميائيون عادةً النسبة المئوية للمردود، والتي تصف نسبة المردود الفعلي إلى المردود النظري. ويتم حسابها على النحو التالي:

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

Percent yields may range from a fraction of 1 percent to 100 percent.

قد تتراوح نسبة العائد من جزء من 1% إلى 100%.

- The theoretical yield is the yield that you calculate using the balanced equation.
- The actual yield is the yield obtained by carrying out the reaction.

- الناتج النظري هو الناتج الذي يتم حسابه باستخدام المعادلة الكيميائية الموزونة.
- الناتج الفعلي هو الناتج الذي يتم الحصول عليه من خلال إجراء التفاعل.

EXAMPLE

Titanium is a strong, lightweight, corrosion-resistant metal that is used in rockets, aircraft, jet engines, and bicycle frames. It is prepared by the reaction of titanium(IV) chloride with molten magnesium between 950°C and 1150°C:

$$TiCl_4(g) + 2Mg(l) \longrightarrow Ti(s) + 2MgCl_2(l)$$

In a certain industrial operation 3.54×10^7 g of $TiCl_4$ are reacted with 1.13×10^7 g of Mg.

(a) Calculate the theoretical yield of Ti in grams.

(b) Calculate the percent yield if 7.91×10^6 g of Ti are actually obtained.

Because there are two reactants, this is likely to be a **limiting reagent** problem.

(a) from $TiCl_4$

$$\text{moles of Ti} = 3.54 \times 10^7 \cancel{\text{g TiCl}_4} \times \frac{1 \cancel{\text{mol TiCl}_4}}{189.7 \cancel{\text{g TiCl}_4}} \times \frac{1 \text{ mol Ti}}{1 \cancel{\text{mol TiCl}_4}} = 1.87 \times 10^5 \text{ mol Ti}$$

from Mg

$$\text{moles of Ti} = 1.13 \times 10^7 \cancel{\text{g Mg}} \times \frac{1 \cancel{\text{mol Mg}}}{24.31 \cancel{\text{g Mg}}} \times \frac{1 \text{ mol Ti}}{2 \cancel{\text{mol Mg}}} = 2.32 \times 10^5 \text{ mol Ti}$$

Therefore, **$TiCl_4$** is the limiting reagent because it produces a smaller amount of **Ti**. The mass of **Ti** formed is

$$1.87 \times 10^5 \cancel{\text{mol Ti}} \times \frac{47.88 \text{ g Ti}}{1 \cancel{\text{mol Ti}}} = 8.95 \times 10^6 \text{ g Ti}$$

(b) The mass of Ti determined in part (a) is the theoretical yield. The amount given in part (b) is the actual yield of the reaction.

$$\begin{aligned}\% \text{yield} &= \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\% \\ &= \frac{7.91 \times 10^6 \text{ g}}{8.95 \times 10^6 \text{ g}} \times 100\% \\ &= 88.4\%\end{aligned}$$