Chemistry, Raymond Chang
10th edition, 2010
McGraw-Hill

Chapter 3

Mass Relationships in Chemical Reactions

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3.1
Atomic Mass

Atomic Mass

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

Knowledge of an atom's mass is important in laboratory work;

Micro World
(atoms & molecules)

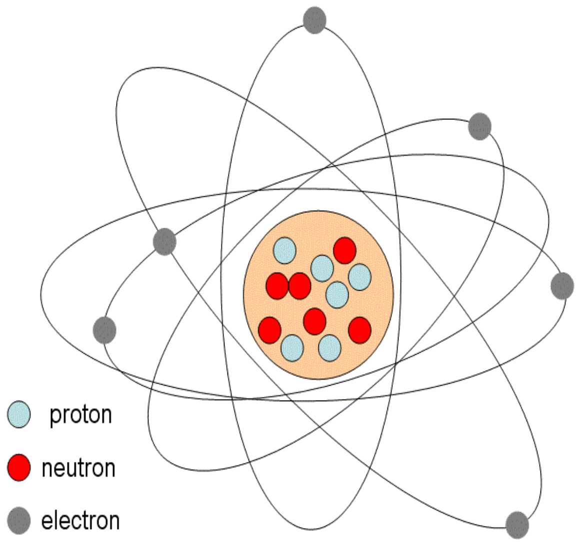
Macro World
(grams)

We cannot weigh a single atom, but it is possible to determine the mass of one atom relative to another experimentally. The first step is to assign a value to the mass of one atom of a given element so that it can be used as a standard.

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

By definition and international agreement: one atomic mass unit is defined as a mass exactly equal to one-twelfth the mass of one carbon-12 atom.

Setting the atomic mass of carbon-12 at 12 amu provides the **standard** for measuring the atomic mass of the other elements.



6 p, 6 e, 6 n

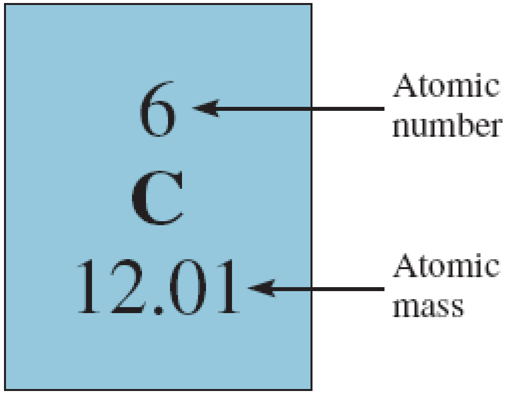
e.g., experiments have shown that, on average, a hydrogen atom is only 8.400 percent as massive as the carbon-12 atom. Thus, if the mass of one carbon-12 atom is exactly 12 amu, the atomic mass of hydrogen must be

(**0.084 x 12.00 amu = 1.008 amu**)

Similar calculations show that the atomic mass of iron is 55.85 amu. Thus, although we do not know just how much an average iron atom's mass is, we know that it is approximately 56 times as massive as a hydrogen atom.

Average Atomic Mass

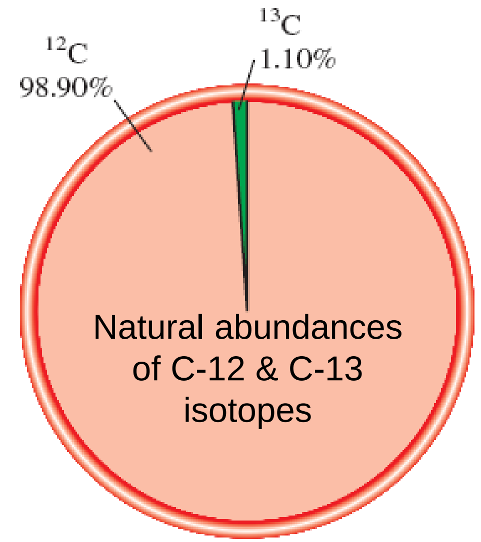
The atomic mass of carbon in a periodic table is not 12.00 amu but 12.01 amu. The reason for the difference is that most naturally occurring elements (including carbon) have more than one isotope.



This means that when we measure the atomic mass of an element, we must generally settle for the **average mass** of the naturally occurring mixture of isotopes.

Note: The atomic mass of an element is based on the average mass of the stable (nonradioactive) isotopes of the element.

e.g., the natural abundances of carbon-12 and carbon-13 are 98.90 percent and 1.10 percent, respectively. The atomic mass of carbon-13 has been determined to be 13.00335 amu. Thus, the average atomic mass of carbon can be calculated as follows:



average atomic mass of natural carbon

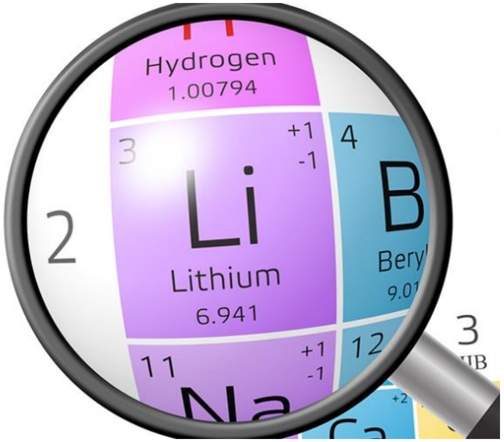
$$= (0.9890)(12.00000\text{ amu}) + (0.0110)(13.00335\text{ amu})$$

$$= 12.01\text{ amu}$$

Naturally occurring lithium is:

7.42% ^{6}Li (6.015 amu)

92.58% ^{7}Li (7.016 amu)



Average atomic mass of lithium =

$$\frac{7.42 \times 6.015 + 92.58 \times 7.016}{100} = 6.941\text{ amu}$$

EXAMPLE

Copper, a metal known since ancient times, is used in electrical cables and pennies, among other things. The atomic masses of its two stable isotopes, ${}^{63}_{29}Cu$ (69.09 percent) and ${}^{65}_{29}Cu$ (30.91 percent), are 62.93 amu and 64.9278 amu, respectively. Calculate the average atomic mass of copper. The relative abundances are given in parentheses.

Solution

Each isotope contributes to the average atomic mass based on its relative abundance.

(0.6909)(62.93 amu) + (0.3091)(64.9278 amu) = 63.55 amu

Practice Exercise

The atomic masses of the two stable isotopes of boron, ${}^{10}_{5}B$ (19.78 percent) and ${}^{11}_{5}B$ (80.22 percent), are 10.0129 amu and 11.0093 amu, respectively. Calculate the average atomic mass of boron.

3.2
Avogadro's Number and Molar Mass of an Element

Mole

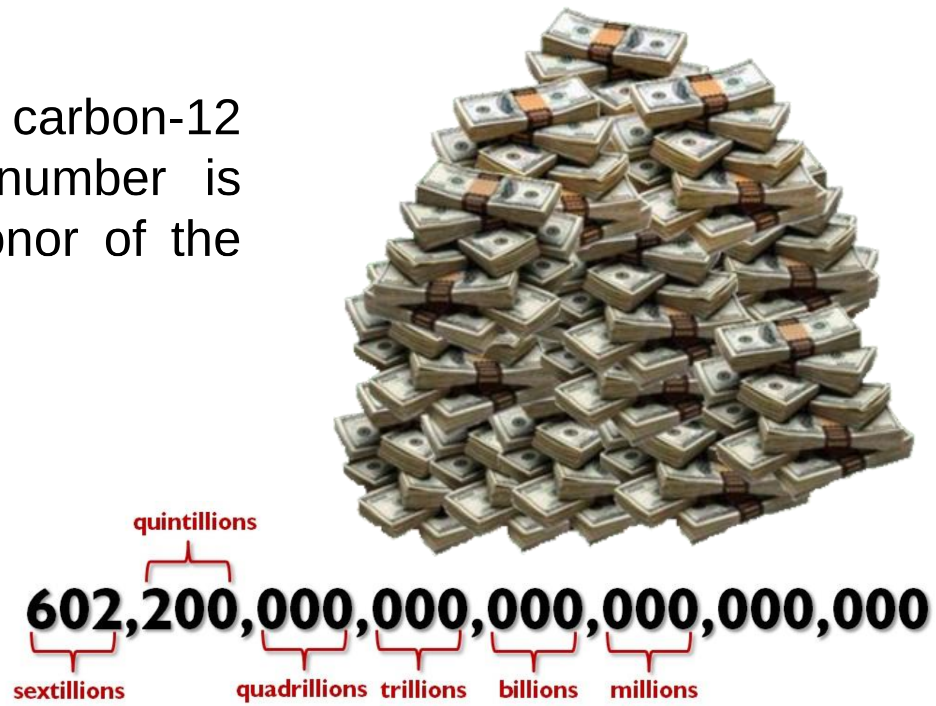
Chemists measure atoms and molecules in **moles**.

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 (or 0.012 kg) of the carbon-12 isotope.

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**.

The currently accepted value is:

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



Because atoms and molecules are so tiny, we need a huge number to study them in manageable quantities.

One mole each of several common elements. Carbon (black charcoal powder), sulfur (yellow powder), iron (as nails), copper wires, and mercury (shiny liquid metal).

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 SO_4^{2-} **ions** contains 6.022 x 10^{23} SO_4^{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 6.022×10^{23} atoms. This mass of C-12 is its **molar mass ($\mathcal{M}$),** defined as the mass (in grams or kilograms) 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.

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

Knowing the molar mass and Avogadro's number, we can calculate the mass of a single atom in grams.

e.g., we know the molar mass of carbon-12 is 12.00 g; therefore, the mass of one carbon-12 atom is given by:

$$\frac{12.00 \text{ g carbon-12 atoms}}{6.022 \times 10^{23} \text{ carbon-12 atoms}} = 1.993 \times 10^{-23} \text{ g}$$

We can use the preceding result to determine the relationship between atomic mass units and grams.

Because the mass of every carbon-12 atom is exactly 12 amu, the number of atomic mass units equivalent to 1 gram is

$$\frac{\text{amu}}{\text{gram}} = \frac{12\ \text{amu}}{1\ \cancel{\text{carbon-12 atom}}} \times \frac{1\ \cancel{\text{carbon-12 atom}}}{1.993 \times 10^{-23}\ \text{g}} = 6.022 \times 10^{23}\ \text{amu/g}$$

Thus,

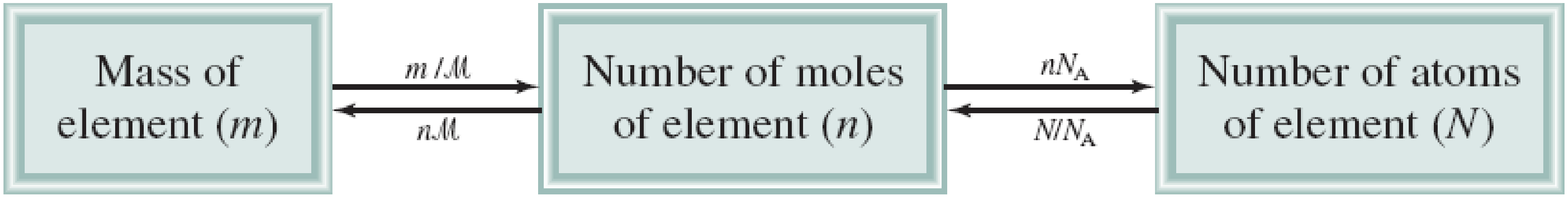
$$1\ \text{g} = 6.022 \times 10^{23}\ \text{amu}$$

and

$$1\ \text{amu} = 1.661 \times 10^{-24}\ \text{g}$$

This example shows that Avogadro's number can be used to convert from the atomic mass units to mass in grams and vice versa.

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



$$n = \frac{m}{\mathcal{M}} \qquad N_A = \frac{N}{n}$$

N_A : Avogadro's no. = 6.022 x 10^{23}

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?

1 mol He = 4.003 g He (from periodic table)

Thus, we can write two conversion factors:

$$\frac{1 \text{ mol He}}{4.003 \text{ g He}} \quad \text{and} \quad \frac{4.003 \text{ g He}}{1 \text{ mol He}}$$

The conversion factor on the left is the correct one. Grams will cancel, leaving the unit mol for the answer, that is,

$$6.46 \cancel{\text{g He}} \times \frac{1 \text{ mol He}}{4.003 \cancel{\text{g He}}} = \boxed{1.61 \text{ mol He}}$$

Practice Exercise

How many moles of magnesium (Mg) are there in 87.3 g of Mg?

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?

1 mol Zn = 65.39 g Zn (from periodic table)

Thus, we can write two conversion factors:

$$\frac{1 \text{ mol Zn}}{65.39 \text{ g Zn}} \quad \text{and} \quad \frac{65.39 \text{ g Zn}}{1 \text{ mol Zn}}$$

The conversion factor on the right is the correct one. Moles will cancel, leaving unit of grams for the answer. The number of grams of Zn is

$$0.356 \cancel{\text{mol Zn}} \times \frac{65.39 \text{ g Zn}}{1 \cancel{\text{mol Zn}}} = \boxed{23.3 \text{ g Zn}}$$

Practice Exercise

Calculate the number of grams of lead (Pb) in 12.4 moles of lead.

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?

$$\text{grams of S} \longrightarrow \text{moles of S} \longrightarrow \text{number of S atoms}$$

1 mol S = 32.07 g S

the conversion factor is $\dfrac{1 \text{ mol S}}{32.07 \text{ g S}}$

1 mol = 6.022 x 10^{23} particles (atoms)

the conversion factors are $\dfrac{6.022 \times 10^{23} \text{ S atoms}}{1 \text{ mol S}}$ and $\dfrac{1 \text{ mol S}}{6.022 \times 10^{23} \text{ S atoms}}$

$$16.3 \cancel{\text{g S}} \times \frac{1 \cancel{\text{mol S}}}{32.07 \cancel{\text{g S}}} \times \frac{6.022 \times 10^{23} \text{ S atoms}}{1 \cancel{\text{mol S}}} = \boxed{3.06 \times 10^{23} \text{ S atoms}}$$

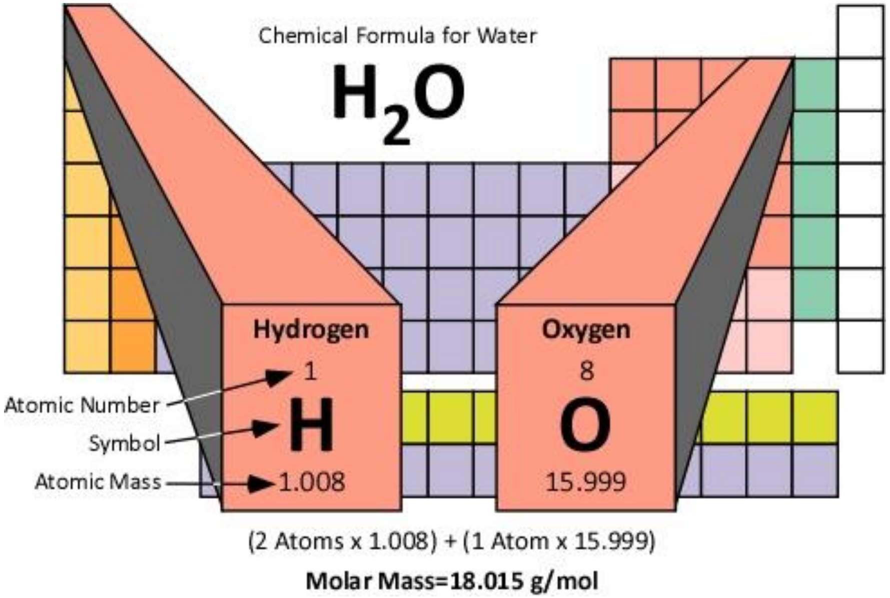
Practice Exercise

Calculate the number of atoms in 0.551 g of potassium (K).

3.3
Molecular Mass

If we know the atomic masses of the component atoms, we can calculate the mass of a molecule.

The **molecular mass** (sometimes called molecular weight) is the sum of the atomic masses (in amu) in the molecule.



e.g., the molecular mass of $\mathbf{H_2O}$ is

2 (atomic mass of H) + 1 (atomic mass of O)

or 2 (1.008) + (15.999) = 18.015 amu

EXAMPLE

Calculate the molecular masses (in amu) of the following compounds:

(a) Sulfur dioxide (SO_2) and
(b) Caffeine ($C_8H_{10}N_4O_2$).

(a) molecular mass of SO_2 = 32.07 + 2(16.00)
= 64.07 amu

(b) molecular mass of $C_8H_{10}N_4O_2$ =
8(12.01) + 10(1.008) + 4(14.01) + 2(16.00) = 194.20 amu

Practice Exercise

What is the molecular mass of methanol (CH_4O)?

EXAMPLE

Methane (CH_4) is the principal component of natural gas. How many moles of CH_4 are present in 6.07 g of CH_4?

molar mass of CH_4 = 12.01 + 4(1.008) = 16.04 g

1 mol CH_4 = 16.04 g CH_4

The conversion factor:

$$\frac{1 \text{ mol } CH_4}{16.04 \text{ g } CH_4}$$

$$6.07\ \cancel{\text{g } CH_4} \times \frac{1 \text{ mol } CH_4}{16.04\ \cancel{\text{g } CH_4}} = \boxed{0.378 \text{ mol } CH_4}$$

Practice Exercise

Calculate the number of moles of chloroform ($CHCl_3$) in 198 g of chloroform.

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.

$$\text{grams of urea} \longrightarrow \text{moles of urea} \longrightarrow \text{moles of H} \longrightarrow \text{atoms of H}$$

$$25.6\ \cancel{\text{g}\ (\text{NH}_2)_2\text{CO}} \times \frac{1\ \cancel{\text{mol}\ (\text{NH}_2)_2\text{CO}}}{60.06\ \cancel{\text{g}\ (\text{NH}_2)_2\text{CO}}} \times \frac{4\ \cancel{\text{mol H}}}{1\ \cancel{\text{mol}\ (\text{NH}_2)_2\text{CO}}} \times \frac{6.022 \times 10^{23}\ \text{H atoms}}{1\ \cancel{\text{mol H}}}$$

$= 1.03 \times 10^{24}$ H atoms

Practice Exercise

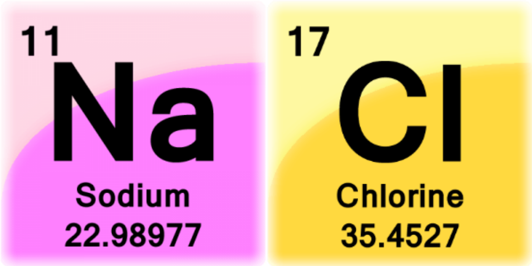
How many H atoms are in 72.5 g of isopropanol (rubbing alcohol), C_3H_8O?

For ionic compounds like NaCl, MgO and $CaCl_2$ that do not contain discrete molecular units, we use the term **formula mass** instead.

e.g., the formula unit of NaCl consists of one Na^+ ion and one Cl^- ion.

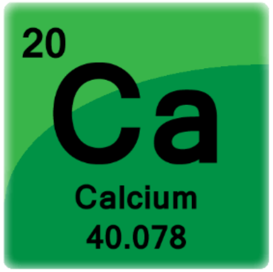
Thus, the formula mass of NaCl is the mass of one formula unit:

formula mass of NaCl = 22.99 amu + 35.45 amu
= 58.44 amu



and its molar mass is 58.44 g.

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



3.5
Percent Composition of Compounds

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

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

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

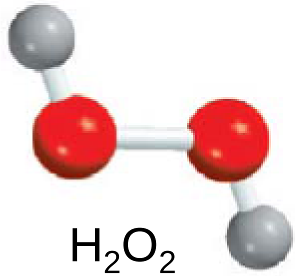
where *n* is the number of moles of the element in 1 mole of the compound.

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:

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

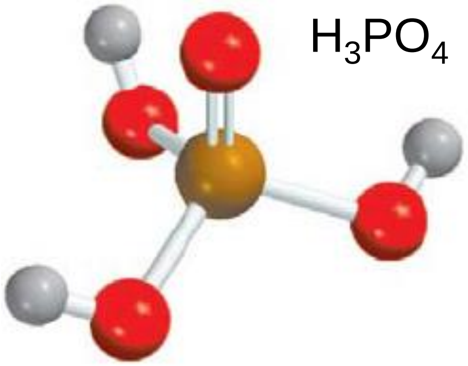
$$\%\text{O} = \frac{2 \times 16.00 \text{ g O}}{34.02 \text{ g H}_2\text{O}_2} \times 100\% = 94.06\%$$



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.

$$\%\text{H} = \frac{3(1.008\text{ g})\text{ H}}{97.99\text{ g H}_3\text{PO}_4} \times 100\% = \boxed{3.086\%}$$

$$\%\text{P} = \frac{30.97\text{ g P}}{97.99\text{ g H}_3\text{PO}_4} \times 100\% = \boxed{31.61\%}$$

$$\%\text{O} = \frac{4(16.00\text{ g})\text{ O}}{97.99\text{ g H}_3\text{PO}_4} \times 100\% = \boxed{65.31\%}$$

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

Practice Exercise

Calculate the percent composition by mass of each of the elements in sulfuric acid (H_2SO_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.

If 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.

$$n_C = 40.92\ \cancel{g\ C} \times \frac{1\ \text{mol C}}{12.01\ \cancel{g\ C}} = 3.407\ \text{mol C}$$

$$n_H = 4.58\ \cancel{g\ H} \times \frac{1\ \text{mol H}}{1.008\ \cancel{g\ H}} = 4.54\ \text{mol H}$$

$$n_O = 54.50\ \cancel{g\ O} \times \frac{1\ \text{mol O}}{16.00\ \cancel{g\ O}} = 3.406\ \text{mol O}$$

We arrive at the formula $\mathbf{C_{3.407}H_{4.54}O_{3.406}}$, which gives the identity and the mole ratios of atoms present. However, chemical formulas are written with whole numbers.

$$\text{C:}\ \frac{3.407}{3.406} \approx 1$$

$$\text{H:}\ \frac{4.54}{3.406} = 1.33$$

$$\text{O:}\ \frac{3.406}{3.406} = 1$$

This gives $\mathbf{CH_{1.33}O}$ as the formula for ascorbic acid. Next, we need to convert 1.33, the subscript for H, into an integer.

$$1.33 \times 1 = 1.33$$
$$1.33 \times 2 = 2.66$$
$$1.33 \times 3 = 3.99 \approx 4$$

Because 1.33 x 3 gives us an integer 4, we multiply all the subscripts by 3 and obtain $\mathbf{C_3H_4O_3}$ as the empirical formula for ascorbic acid.

Practice Exercise

Determine the empirical formula of a compound having the following percent composition by mass: K: 24.75 percent; Mn: 34.77 percent; O: 40.51 percent.

EXAMPLE

Chalcopyrite ($CuFeS_2$) is a principal mineral of copper. Calculate the number of kilograms of Cu in 3.71 x 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

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

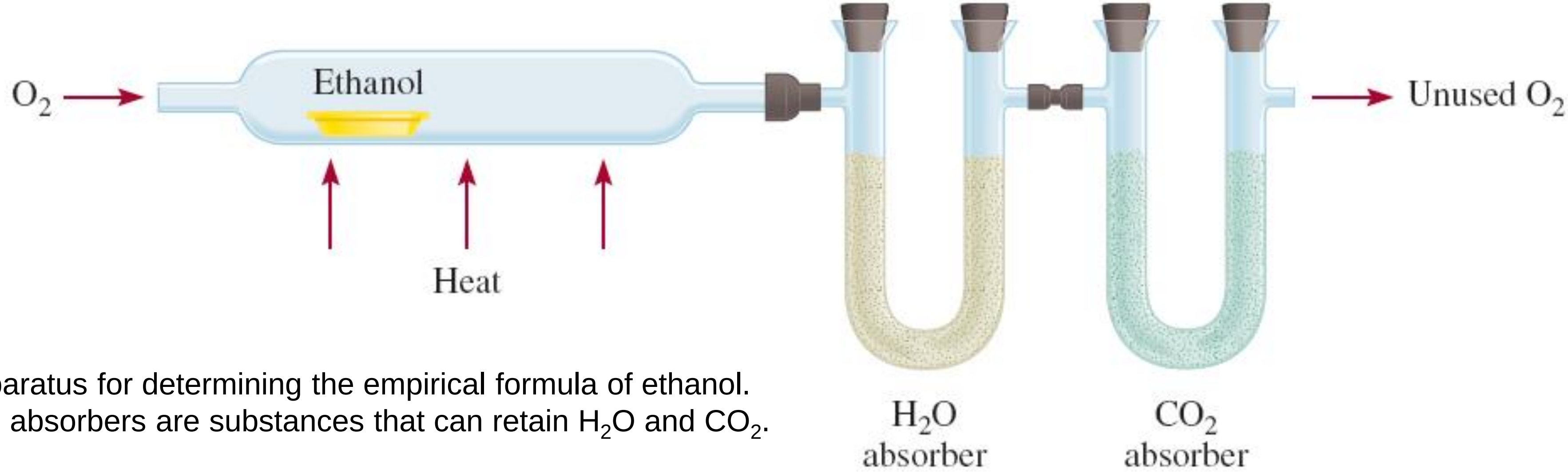
To calculate the mass of Cu in a 3.71 x 10^3 kg sample of $CuFeS_2$, we need to convert the percentage to a fraction (that is, convert 34.63 percent to 34.63/100, or 0.3463) and write

mass of Cu in $CuFeS_2$ = 0.3463 x (3.71 x 10^3 kg) = 1.28 x 10^3 kg

Practice Exercise

Calculate the number of grams of Al in 371 g of Al_2O_3.

3.6
Experimental Determination of Empirical Formulas



Apparatus for determining the empirical formula of ethanol.
The absorbers are substances that can retain H_2O and CO_2.

When ethanol is burned in an apparatus, CO_2 and H_2O are given off. Because neither carbon (C) nor hydrogen (H) was in the inlet gas, we can conclude that both C & H were present in ethanol and that oxygen (O) may also be present. Molecular oxygen (O_2) was added in the combustion process, but some O may also have come from the original ethanol sample.

The masses of CO_2 and of H_2O produced can be determined by measuring the increase in mass of the CO_2 and H_2O absorbers, respectively.

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:

$$\text{mass of C} = 22.0\ \cancel{\text{g CO}_2} \times \frac{1\ \cancel{\text{mol CO}_2}}{44.01\ \cancel{\text{g CO}_2}} \times \frac{1\ \cancel{\text{mol C}}}{1\ \cancel{\text{mol CO}_2}} \times \frac{12.01\ \text{g C}}{1\ \cancel{\text{mol C}}}$$
$$= 6.00\ \text{g C}$$

$$\text{mass of H} = 13.5\ \cancel{\text{g H}_2\text{O}} \times \frac{1\ \cancel{\text{mol H}_2\text{O}}}{18.02\ \cancel{\text{g H}_2\text{O}}} \times \frac{2\ \cancel{\text{mol H}}}{1\ \cancel{\text{mol H}_2\text{O}}} \times \frac{1.008\ \text{g H}}{1\ \cancel{\text{mol H}}}$$
$$= 1.51\ \text{g H}$$

Thus, 11.5 g of ethanol contains 6.00 g of carbon and 1.51 g of hydrogen. The remainder must be oxygen, whose mass is

$$\begin{aligned} \text{mass of O} &= \text{mass of sample} - (\text{mass of C} + \text{mass of H}) \\ &= 11.5\ \text{g} - (6.00\ \text{g} + 1.51\ \text{g}) \\ &= 4.0\ \text{g} \end{aligned}$$

The number of moles of each element present in 11.5 g of ethanol is

$$\text{moles of C} = 6.00\ \cancel{\text{g C}} \times \frac{1\ \text{mol C}}{12.01\ \cancel{\text{g C}}} = 0.500\ \text{mol C}$$

$$\text{moles of H} = 1.51\ \cancel{\text{g H}} \times \frac{1\ \text{mol H}}{1.008\ \cancel{\text{g H}}} = 1.50\ \text{mol H}$$

$$\text{moles of O} = 4.0\ \cancel{\text{g O}} \times \frac{1\ \text{mol O}}{16.00\ \cancel{\text{g O}}} = 0.25\ \text{mol O}$$

The formula of ethanol is therefore $\mathbf{C_{0.50}H_{1.5}O_{0.25}}$. Because the number of atoms must be an integer, we divide the subscripts by 0.25, the smallest subscript, and obtain for the empirical formula $\mathbf{C_2H_6O}$.

Molecular formula from empirical formula

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.

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

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

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 between 90 g and 95 g. Determine the molecular formula and the accurate molar mass of the compound.

$$n_N = 1.52\ \cancel{\text{g N}} \times \frac{1\ \text{mol N}}{14.01\ \cancel{\text{g N}}} = 0.108\ \text{mol N}$$

$$n_O = 3.47\ \cancel{\text{g O}} \times \frac{1\ \text{mol O}}{16.00\ \cancel{\text{g O}}} = 0.217\ \text{mol O}$$

We arrive at the formula $\mathbf{N_{0.108}O_{0.217}}$. By dividing the subscripts by the smaller subscript (0.108), we obtain $\mathbf{NO_2}$ as the empirical formula.

Empirical molar mass = 14.01 g + 2(16.00 g) = 46.01 g

Next, we determine the ratio between the molar mass and the empirical molar mass

$$\frac{\text{molar mass}}{\text{empirical molar mass}} = \frac{90\ \text{g}}{46.01\ \text{g}} \approx 2$$

The molar mass is twice the empirical molar mass. This means that there are two NO_2 units in each molecule, and the molecular formula is $(NO_2)_2$ or $\mathbf{N_2O_4}$.

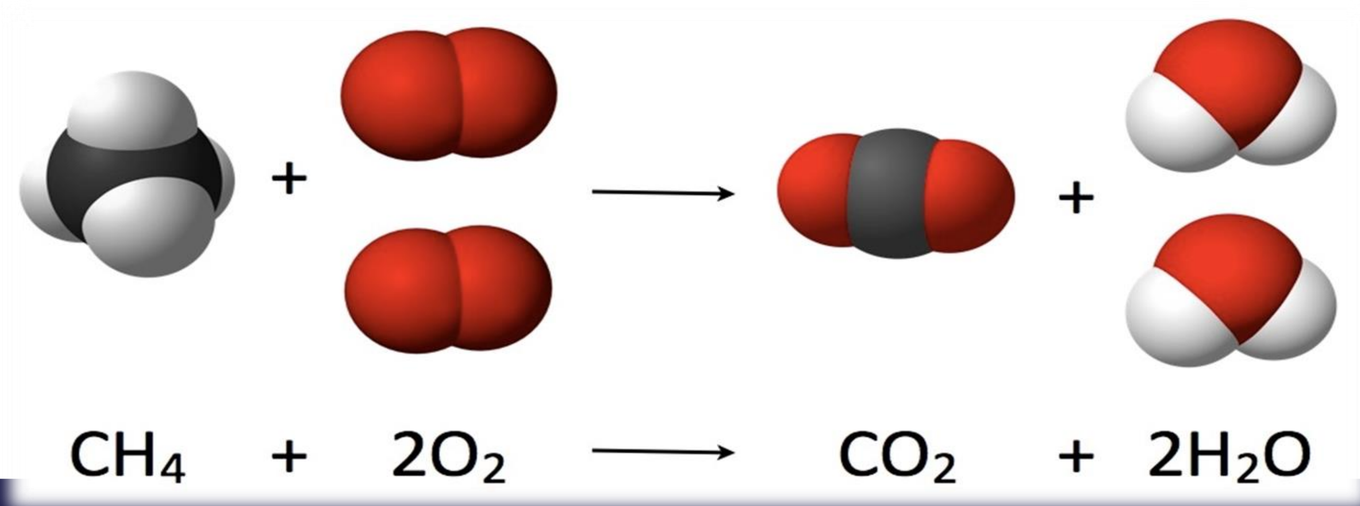
Practice Exercise

A sample of a compound containing boron (B) and hydrogen (H) contains 6.444 g of B and 1.803 g of H. The molar mass of the compound is about 30 g. What is its molecular formula?

3.7
Chemical Reactions and Chemical Equations

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

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



Writing Chemical Equations

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"

$\longrightarrow$ 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).

$$2H_2 + O_2 \longrightarrow 2H_2O$$ (balanced equation)

$$\begin{array}{lll}
2H_2 & + \; O_2 & \longrightarrow 2H_2O \\
\text{Two molecules} & + \; \text{one molecule} & \longrightarrow \text{two molecules} \\
2 \text{ moles} & + \; 1 \text{ mole} & \longrightarrow 2 \text{ moles} \\
\multicolumn{2}{l}{\underbrace{2(2.02 \text{ g}) = 4.04 \text{ g} + 32.00 \text{ g}}_{36.04 \text{ g reactants}}} & \longrightarrow \underbrace{2(18.02 \text{ g}) = 36.04 \text{ g}}_{36.04 \text{ g product}}
\end{array}$$

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

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.

Products appear on the right side of the equation.

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.

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

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.

Balancing Chemical Equations

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

$$KClO_3 \longrightarrow KCl + O_2$$

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

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

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

Check the number of each element

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

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.

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

$$C_2H_6 + O_2 \longrightarrow 2CO_2 + H_2O$$

$$C_2H_6 + O_2 \longrightarrow 2CO_2 + 3H_2O$$

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

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.

$$Al + O_2 \longrightarrow Al_2O_3$$

$$2Al + O_2 \longrightarrow Al_2O_3$$

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

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

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

3.8
Amounts of Reactants and Products

Stoichiometry

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

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

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

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

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

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

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
6.022×10^{23} molecules		$3(6.022 \times 10^{23}$ molecules)		$2(6.022 \times 10^{23}$ 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".

This relationship enables us to write the conversion factors

$$\frac{3 \text{ mol } H_2}{2 \text{ mol } NH_3} \quad \text{and} \quad \frac{2 \text{ mol } NH_3}{3 \text{ mol } H_2}$$

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

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?

$$\begin{aligned}\text{moles of } NH_3 \text{ produced} &= 6.0\ \cancel{\text{mol } H_2} \times \frac{2 \text{ mol } NH_3}{3\ \cancel{\text{mol } H_2}} \\ &= 4.0 \text{ mol } NH_3\end{aligned}$$

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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?

the link between H_2 and NH_3 is the mole ratio from the balanced equation. So we need to first convert grams of H_2 to moles of H_2, then to moles of NH_3, and finally to grams of NH_3.

$$\begin{aligned}\text{moles of } H_2 &= 16.0\ \cancel{\text{g } H_2} \times \frac{1 \text{ mol } H_2}{2.016\ \cancel{\text{g } H_2}} \\ &= 7.94 \text{ mol } H_2\end{aligned} \Bigg/ \begin{aligned}\text{moles of } NH_3 &= 7.94\ \cancel{\text{mol } H_2} \times \frac{2 \text{ mol } NH_3}{3\ \cancel{\text{mol } H_2}} \\ &= 5.29 \text{ mol } NH_3\end{aligned} \Bigg/ \begin{aligned}\text{grams of } NH_3 &= 5.29\ \cancel{\text{mol } NH_3} \times \frac{17.03 \text{ g } NH_3}{1\ \cancel{\text{mol } NH_3}} \\ &= 90.1 \text{ g } NH_3\end{aligned}$$

$$\begin{aligned}\text{grams of } NH_3 &= 16.0\ \cancel{\text{g } H_2} \times \frac{1\ \cancel{\text{mol } H_2}}{2.016\ \cancel{\text{g } H_2}} \times \frac{2\ \cancel{\text{mol } NH_3}}{3\ \cancel{\text{mol } H_2}} \times \frac{17.03 \text{ g } NH_3}{1\ \cancel{\text{mol } NH_3}} \\ &= 90.1 \text{ g } NH_3\end{aligned}$$

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

$$\begin{aligned}\text{grams of } N_2 &= 16.0\ \cancel{\text{g } H_2} \times \frac{1\ \cancel{\text{mol } H_2}}{2.016\ \cancel{\text{g } H_2}} \times \frac{1\ \cancel{\text{mol } N_2}}{3\ \cancel{\text{mol } H_2}} \times \frac{28.02 \text{ g } N_2}{1\ \cancel{\text{mol } N_2}} \\ &= 74.1 \text{ g } N_2\end{aligned}$$

EXAMPLE

The food we eat is degraded, or broken down, in our bodies to provide energy for growth and function. A general overall equation for this very complex process represents the degradation of glucose ($C_6H_{12}O_6$) to carbon dioxide (CO_2) and water (H_2O):

$$C_6H_{12}O_6 + 6O_2 \longrightarrow 6CO_2 + 6H_2O$$

If 856 g of $C_6H_{12}O_6$ is consumed by a person over a certain period, what is the mass of CO_2 produced?

$$\text{grams of } C_6H_{12}O_6 \longrightarrow \text{moles of } C_6H_{12}O_6 \longrightarrow \text{moles of } CO_2 \longrightarrow \text{grams of } CO_2$$

$$856\ \cancel{\text{g } C_6H_{12}O_6} \times \frac{1 \text{ mol } C_6H_{12}O_6}{180.2\ \cancel{\text{g } C_6H_{12}O_6}} = 4.750 \text{ mol } C_6H_{12}O_6$$

$$4.750\ \cancel{\text{mol } C_6H_{12}O_6} \times \frac{6 \text{ mol } CO_2}{1\ \cancel{\text{mol } C_6H_{12}O_6}} = 28.50 \text{ mol } CO_2$$

$$28.50\ \cancel{\text{mol } CO_2} \times \frac{44.01 \text{ g } CO_2}{1\ \cancel{\text{mol } CO_2}} = 1.25 \times 10^3 \text{ g } CO_2$$

$$\text{mass of } CO_2 = 856\ \cancel{\text{g } C_6H_{12}O_6} \times \frac{1\ \cancel{\text{mol } C_6H_{12}O_6}}{180.2\ \cancel{\text{g } C_6H_{12}O_6}} \times \frac{6\ \cancel{\text{mol } CO_2}}{1\ \cancel{\text{mol } C_6H_{12}O_6}} \times \frac{44.01 \text{ g } CO_2}{1\ \cancel{\text{mol } CO_2}}$$
$$= \boxed{1.25 \times 10^3 \text{ g } CO_2}$$

EXAMPLE

All alkali metals react with water to produce hydrogen gas and the corresponding alkali metal hydroxide. A typical reaction is that between lithium and water:

$$2\mathrm{Li}(s) + 2\mathrm{H_2O}(l) \longrightarrow 2\mathrm{LiOH}(aq) + \mathrm{H_2}(g)$$

How many grams of Li are needed to produce 9.89 g of H_2?

$$\text{grams of } \mathrm{H_2} \longrightarrow \text{moles of } \mathrm{H_2} \longrightarrow \text{moles of Li} \longrightarrow \text{grams of Li}$$

$$9.89\ \cancel{\mathrm{g\ H_2}} \times \frac{1\ \cancel{\mathrm{mol\ H_2}}}{2.016\ \cancel{\mathrm{g\ H_2}}} \times \frac{2\ \cancel{\mathrm{mol\ Li}}}{1\ \cancel{\mathrm{mol\ H_2}}} \times \frac{6.941\ \mathrm{g\ Li}}{1\ \cancel{\mathrm{mol\ Li}}} = \boxed{68.1\ \mathrm{g\ Li}}$$

Practice Exercise

Methanol (CH_3OH) burns in air according to the equation

$$2CH_3OH + 3O_2 \longrightarrow 2CO_2 + 4H_2O$$

If 209 g of methanol are used up in a combustion process, what is the mass of H_2O produced?

Practice Exercise

The reaction between nitric oxide (NO) and oxygen to form nitrogen dioxide (NO_2) is a key step in photochemical smog formation:

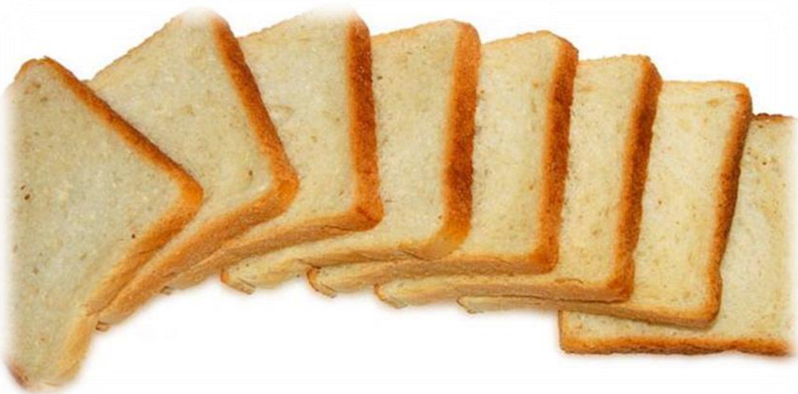
$$2NO(g) + O_2(g) \longrightarrow 2NO_2(g)$$

How many grams of O_2 are needed to produce 2.21 g of NO_2?

3.9
Limiting Reagents

Limiting Reagents

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.

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.

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

EXAMPLE

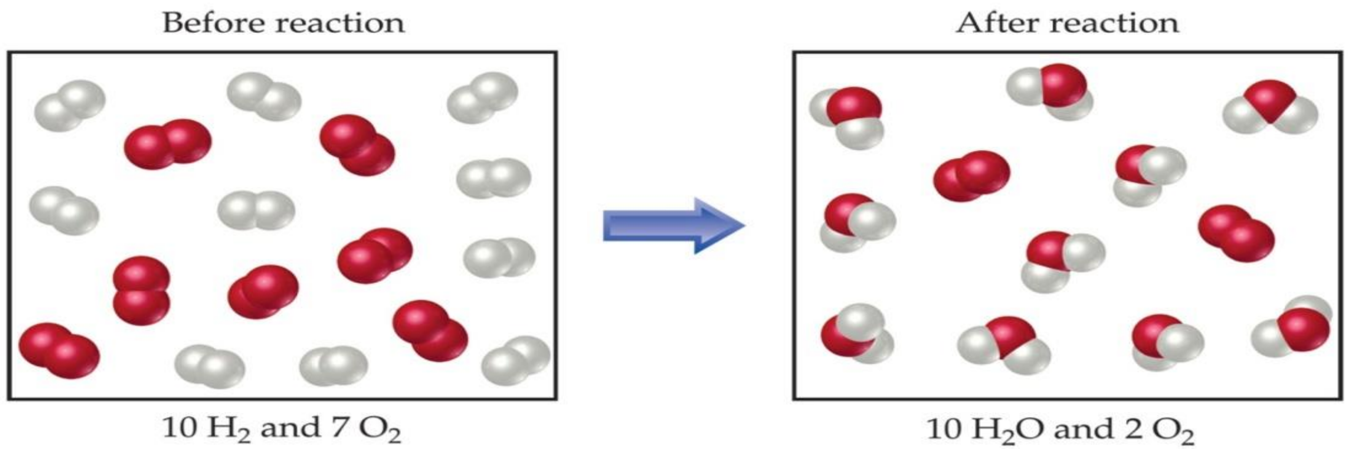
$$2\,H_2(g) + O_2(g) \longrightarrow 2\,H_2O(g)$$

$$2\text{ mol } H_2 \simeq 1\text{ mol } O_2$$

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:

$$\text{Moles } O_2 = (10\ \cancel{\text{mol } H_2})\left(\frac{1\text{ mol } O_2}{2\ \cancel{\text{mol } H_2}}\right) = 5\text{ mol } O_2$$



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.

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

(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

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

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

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

Practice Exercise

The reaction between aluminum and iron(III) oxide can generate temperatures approaching 3000ºC and is used in welding metals:

$$2Al + Fe_2O_3 \longrightarrow Al_2O_3 + 2Fe$$

In one process, 124 g of Al are reacted with 601 g of Fe_2O_3.

(a) Calculate the mass (in grams) of Al_2O_3 formed.

(b) How much of the excess reagent is left at the end of the reaction?

3.10
Reaction Yield

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.

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

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:

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

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

- 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.

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

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

(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.

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

Practice Exercise

Industrially, vanadium metal, which is used in steel alloys, can be obtained by reacting vanadium(V) oxide with calcium at high temperatures:

$$5Ca + V_2O_5 \longrightarrow 5CaO + 2V$$

In one process, 1.54×10^3 g of V_2O_5 react with 1.96×10^3 g of Ca.

(a) Calculate the theoretical yield of V.

(b) Calculate the percent yield if 803 g of V are obtained.


Thank You!