Empirical and Molecular Formulae

Chemical formulae represent the composition of substances.

The formula of carbon dioxide, for example, is CO_2. This tells us that one molecule of carbon dioxide contains twice as many oxygen atoms as carbon atoms.

Chemical formulae in balanced equations can help us to understand chemical reactions on an atomic scale. For example, the following equation tells us that one mole of carbon atoms reacts with two moles of oxygen atoms (one mole of O_2 molecules contains two moles of O atoms) to make one mole of carbon dioxide molecules.

$$C(s) + O_2(g) \longrightarrow CO_2(g)$$

Chemical substances can be represented by different types of formulae including **empirical formulae** and **molecular formulae**.

An **empirical formula** is the simplest whole-number ratio of atoms of each element in a compound.

A **molecular formula** is the actual number of atoms of each element in a molecule of a compound.

The empirical formula and molecular formula of a substance can be the same or different, as shown by the examples below:

Chemical Substance	Molecular Formula	Empirical Formula
water	H_2O	H_2O
methane	CH_4	CH_4
ethane	$C2H_6$	CH_3
ethanoic acid	$C_2H_4O_2$	CH_2O
glucose	$C_6H_{12}O_6$	CH_2O

Methods for determining the empirical and molecular formulae of substances are shown on the following pages.

Determining an Empirical Formula

Elemental compositions of compounds can be determined experimentally. For example, an experiment could show that an oxide of iron consists of 70% iron by mass. This means that 70% of the compound's mass is iron atoms and 30% of the compound's mass is oxygen atoms. The empirical formula of this compound can be deduced following three steps:

Step 1

Find the mass of each element in the compound.

You may be given the mass of each element or the percentage by mass of each element in the compound.

If percentage by mass values are given, calculate the mass of each element that would be present in 100 g of the compound (100 g is a nice round number, but you could use any amount for the mass of the compound because the percentage, and therefore the ratio, of each element will remain the same).

Example	Iron	Oxygen
	70%	30%
	$\frac{70}{100} \times 100$ g	$\frac{30}{100} \times 100$ g
mass =	70 g	30 g

Step 2

Find the number of moles of each element in the compound.

Divide the mass of each element by its relative atomic mass (Ar).

Example	Iron	Oxygen
A_r =	55.8	16.0
moles =	$\frac{70}{55.8} = 1.254...$	$\frac{30}{16.0} = 1.875$

Step 3

Find the simplest whole number ratio.

Divide each number of moles by the smallest number of moles.

If the simplest ratio calculated does not contain whole numbers, multiply all numbers by the same value to convert the ratio to whole numbers.

Example	Iron	Oxygen
simplest ratio =	$\frac{1.254...}{1.254...} = 1.0$	$\frac{1.875}{1.254...} = 1.5$
	$\times 2$	$\times 2$
simplest whole number ratio =	2	3
	The empirical formula is Fe_2O_3.	

Determining a Molecular Formula

If the relative molecular mass (M_r) and the empirical formula of a compound are known, we can deduce the molecular formula of the compound.

For example, an oxide of iron with a M_r of 159.6 g mol^{-1} has the empirical formula Fe_2O_3. The molecular formula of this compound can be deduced as follows:

Step 1

Calculate the mass of one empirical formula unit.

Find the sum of the relative atomic masses (A_r) of each atom in the empirical formula.

e.g. relative mass of one Fe_2O_3 unit

$= (55.8 \times 2) + (16.0 \times 3)$

$= 159.6$

Step 2

Calculate the number of empirical formula units that are present in one molecule of the compound.

$$\textbf{number of empirical formula units} = \frac{M_r}{\textbf{relative mass of one empirical formula unit}}$$

e.g. $\frac{159.6}{159.6} = 1$

So, there is one empirical formula unit in one molecule of this compound.

The molecular formula is also Fe_2O_3.

Example 1

a. **An experiment shows that a hydrocarbon contains 1.20 g of carbon (C) and 0.30 g of hydrogen (H).**

Deduce the empirical formula of the hydrocarbon.

Example	Carbon	Hydrogen
mass =	1.20 g	0.30 g
A_r =	12.0	1.0
moles =	$\frac{1.20}{1.20} = 0.10$	$\frac{0.30}{1.0} = 0.30$
simplest ratio =	$\frac{0.10}{0.10} = 1.0$	$\frac{0.30}{0.10} = 3.0$
simplest whole number ratio =	1	3
The empirical formula of this compound is CH_3.		

b. **The same hydrocarbon has a relative molecular mass (M_r) of 60.0 g mol^{-1}.**

Determine the molecular formula of the hydrocarbon.

relative mass of one CH_3 unit = (12.0 × 1) + (1.0 × 3) = 15.0

number of empirical formula units in one molecule = $\frac{60.0}{15} = 4$

$CH_3 \times 4 \longrightarrow C_4H_{12}$

The molecular formula of this compound is C_4H_{12}.

Example 2

a. **The complete combustion of an unknown hydrocarbon in excess oxygen produced 11.0 g of carbon dioxide (CO_2) and 4.50 g of water (H_2O).**

Determine the empirical formula of the hydrocarbon.

M_r of CO_2 = (12.0 × 1) + (16.0 × 2) = 44.0

moles of CO_2 produced = $\frac{11.0}{44.0}$ = 0.25 moles

So, there were 0.25 moles of C in the original hydrocarbon that underwent complete combustion.

M_r of H_2O = (1.0 × 2) + (16.0 × 1) = 18.0

moles of H_2O produced = $\frac{4.50}{18.0}$ = 0.25 moles

Each mole of H_2O molecules contains two moles of H atoms.

So, there were 0.5 moles of H in the original hydrocarbon that underwent complete combustion.

Example	Carbon	Hydrogen
moles =	0.25	0.5
simplest ratio =	x4	x4
simplest whole number ratio =	1	2
The empirical formula of this compound is CH_2.		