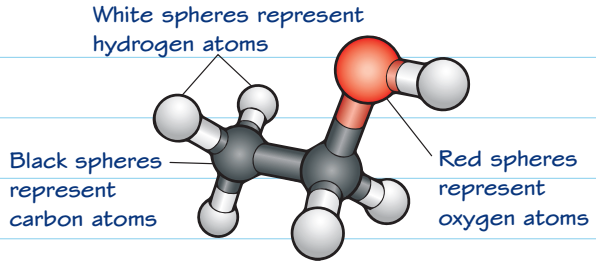
Types of formulae

In simple molecules and giant structures different types of formulae can be used to describe the number or ratio of particles present.

Molecular formulae

Molecular formulae tell you the number and type of each atom in a simple molecule.

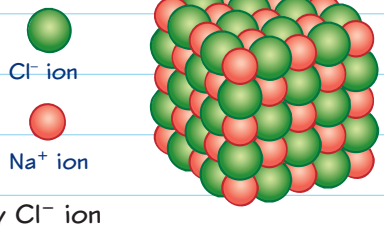


So, in an ethanol molecule there are 2 carbon atoms, 6 hydrogen atoms and 1 oxygen atom. The molecular formula is C_2H_6O.

Empirical formulae

Empirical formulae show the simplest ratio of atoms of different elements in a compound. These are often used to describe the ratios in giant structures as the actual numbers will depend on the amount of the compound.

In sodium chloride there are many ions present in one small grain. There is always one Na^+ ion to every Cl^- ion so the empirical formula is NaCl.



Worked example

A compound is found to contain 4.37 g of nitrogen, 5.00 g of oxygen and 0.63 g of hydrogen, by elemental analysis. It has a relative formula mass of 64.0. Calculate its empirical formula and hence deduce its molecular formula. **(4 marks)**

	Nitrogen	Oxygen	Hydrogen
Amount (mol)	$\frac{4.37}{14.0} = 0.312$	$\frac{5.00}{16.0} = 0.313$	$\frac{0.63}{1.0} = 0.63$
Molar ratio	$\frac{0.312}{0.312} = 1$	$\frac{0.313}{0.312} \approx 1$	$\frac{0.63}{0.312} = 2.02$
Whole number ratio	1	1	2

The empirical formula is NOH_2 with a relative mass of 32.0. The compound's relative formula mass is 64.0, so the molecular formula is double the empirical formula, so $N_2O_2H_4$.

Find the empirical formula by calculating the amount of each element, then divide through by the smallest amount to find the molar ratio. If this is not a whole number ratio scale up as appropriate.

Maths skills This is the smallest amount, so divide the other amounts by this.

Worked example

Using elemental analysis, compound X is found to contain 40.0% C, 6.7% H and 53.3% O. The molar mass of X is 90. Calculate its empirical formula and hence deduce its molecular formula. **(4 marks)**

If analysis data is given as percentages a workaround is to assume you have 100 g of the compound and so consider the percentages as masses. You can then work out the amount in moles.

	Carbon	Hydrogen	Oxygen
Amount (mol)	$\frac{400}{12} = 3.33$	$\frac{6.7}{1} = 6.7$	$\frac{53.3}{16} = 3.33$
Molar ratio	$\frac{3.33}{3.33} = 1$	$\frac{6.7}{3.33} \approx 2$	$\frac{3.33}{3.33} = 1$
Whole number ratio	1	2	1

So the empirical formula is CH_2O. Total atomic masses of the atoms in $CH_2O = 12 + 2 + 16 = 30$.

As the molar mass of X is 9000, which is 3 times bigger, its molecular formula must be 3 times bigger.

Molecular formula of X = $C_3H_6O_3$.

Now try this

An acid is found to contain 0.50 g of hydrogen, 8.18 g of sulfur and 16.3 g of oxygen. Calculate its empirical formula. **(3 marks)**