The Mole Concept

When you go to the supermarket, you may buy a dozen eggs. You may buy a ream of paper for your computer. In everyday life, we have words for a certain number of objects. The same is true of chemistry. Since even the full stop at the end of this sentence contains billions of atoms, we need a term to describe a useful number of atoms. That term is the mole—it comes from the Latin word moles meaning 'a mass'.

The mole

So far we have talked in terms of atoms, ions and molecules, but these are all very small. Chemists need a useful unit to predict the potential yield when treating an ore and to measure the amounts of reactants and products in the laboratory and in industry. A chemical engineer must know the correct mass ratios in reactions in order to produce the highest possible yield of product without wasting any reactant. The mole is a convenient unit and it can be easily converted to grams, number of particles or, in the case of a gas, to volume.

A mole of elements

We have been dealing with elements and so we will start by looking at a mole of some elements.

A mole of gold is the quantity of gold that contains 6.022×10^{23} gold atoms and this would have a mass of 197.0 g.

A mole of sodium is the quantity of sodium that contains 6.022×10^{23} sodium atoms and this would have a mass of 22.99 g.

A mole of iron is the quantity of iron that contains 6.022×10^{23} iron atoms and this would have a mass of 55.85 g.

A mole of sulfur is the quantity of sulfur that contains 6.022×10^{23} sulfur atoms and this would have a mass of 32.06 g.

The masses mentioned, in grams, are the atomic masses of the elements, from the periodic table. The number 6.022×10^{23} is called Avogadro's constant (N_A) Notice that 1 mole of gold contains the same number of atoms as 1 mole of sodium, but a mole of gold weighs a lot more than a mole of sodium. This tells us that gold atoms must be much heavier than those of sodium. Before we look at more complex chemicals, think about something more obvious .... a mole of cars.

A mole of cars would contain 6.022×10^{23} cars. If each car has 2 headlights, then a mole of cars would have 2 moles of headlights altogether, that is 12.044×10^{23} headlights. Diatomic molecules are like this. Oxygen gas exists as diatomic molecules, each molecule having 2 atoms. So a mole of oxygen (O_2) contains 6.022×10^{23} oxygen molecules and thus 12.044×10^{23} oxygen atoms. The mass of a mole of oxygen atoms (O) is 16 g so the mass of a mole of oxygen gas (O_2) is 32 g.

A mole of a compound

We can also measure a mole of a compound. A mole of water (H_2O) contains 6.022×10^{23} molecules of water and is made of 2 moles of hydrogen atoms (12.044×10^{23} atoms) and 1 mole of oxygen atoms (6.022×10^{23} atoms). A mole of water also has a mass of 18.016 g (2.016 + 16). To find the molar mass of a compound, you just add the atomic masses of the atoms that make up the compound. This is also sometimes called the formula mass of a compound. One mole of sodium chloride (NaCI) contains 6.022×10^{23} formula units of sodium chloride. Thus it contains 6.022×10^{23} sodium ions (Na^+) and 6.022×10^{23} chloride ions (Cl^-). The mass of 1 mole (molar mass) of sodium chloride is 58.44 g (22.99 + 35.45).

Formal Definitions.

A mole is the number of atoms present in exactly 12 of the isotope carbon-12. In 12 g of carbon-12 there are 6.022×10^{23} carbon atoms. So the amount of any other substance that has 6.022×10^{23} particles (atoms ions or molecules) is also a mole. A mole weighs the same as the atomic mass of an element or the formula mass of a compound in grams. The mass of 1 mole of a substance in grams is called the molar mass (M) Notice that mole is sometimes abbreviated to mol.

Avogadro's constant (N_A) is the number of atoms ions or molecules in a mole of a substance. There are 6.022×10^{23} particles in a mole of any substance. This is a lot of particles. 6.022×10^{23} particles of sand grains would cover Australia about 1 m deep in sand If you counted out a mole of anything at the rate of 100 per minute, it would take you 10^{16} years, which is longer than the Earth has existed!

Calculating number of moles

To calculate the number of moles you have of a substance, you divide the mass in grams by the mass of 1 mole (molar mass) of the substance. Always use the information as it is given, for example, if the atomic mass is given as 24.31 g, do not round it off to 24.3 g. In chemical calculations you should never round off until right at the last line of any problem.

$$\text{Number of moles} = \frac{\text{mass}}{\text{Molar mass}}$$

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

Examples

1. Find the molar mass of
   (a) calcium

   (b)nitrogen gas

   (c) magnesium sulfate. Solution

Solution

(a) From the periodic table we find the molar mass of calcium is 40.08 g.

(b) From the periodic table, one mole of nitrogen atoms has a mass of 14.01 g. But nitrogen gas exists as diatomic molecules (N_2). Thus one mole of nitrogen gas has a mass of 2 x 14.01 g.

   Molar mass of N_2 = 2 x 14.01 = 28.02 g

(c) We look up the molar mass of each element in magnesium sulfate and then add them up: Molar mass of $MgSO_4$ = 24.31 + 32.06 + 4 x 16.00 = 120.37 g

2. Calculate the number of moles of copper present in a sample with a mass of 254.20 g.

Solution

To calculate the number of moles of copper, we divide the mass of copper in the sample by the mass of one mole of copper (obtained from the periodic table):

$$n = \frac{m}{M} \qquad \frac{254.20}{63.55} \qquad = 4.00 \text{ moles}$$

3. Calculate the number of moles of magnesium sulfate in a sample, which has a mass of 361.11 g.

Solution

To find the number of moles we divide the mass of magnesium sulfate by its molar mass. From question 1 (c) we know the molar mass is 120.37.

m 361.11

n = $\overline{\quad M \quad}$ $\overline{\quad 120.37 \quad}$ = 3.00 moles

Calculating number of particles

To calculate the number of particles present in a sample of an element or compound you need to use Avogadro's constant. You will not be expected to memorise this number—it will always be given in tests and exams, but you do have to be able to use it. Avogadro's constant tells us that 1 mole of any substance contains 6.022×10^{23} particles — and remember, they can be atoms, ions or molecules. You might be asked to calculate the number of atoms in an element or a compound, the ions in an ionic compound, or the molecules in a substance with covalent bonds. Here are some sample questions worked out.

Examples

1. Calculate the number of

(a) iron atoms in 0.5 moles of sulfur
(b) oxygen molecules in 0.43 moles of hydrogen gas
(c) oxygen atoms in 0.43 moles of hydrogen gas
(d) chloride ions in 6.0 moles of sodium chloride
(e) chloride ions in 6.0 moles of calcium chloride.

Solution

(a) We know that 1 mole of sulfur contains 6.022×10^{23} atoms.

Thus 0.5 moles contains $0.5 \times 6.022 \times 10^{23} = 3.01 \times 10^{23}$ atoms.

(b) We know that 1 mole of hydrogen gas contains 6.022×10^{23} molecules.

Thus 0.43 moles of hydrogen gas contains $0.43 \times 6.022 \times 10^{23} = 2.59 \times 10^{23}$ molecules.

(c) 1 mole hydrogen gas has 2 moles of hydrogen atoms present as oxygen exists as a diatomic molecule (O_2).

Thus 0.43 moles of hydrogen gas contains $2 \times 0.43 \times 6.022 \times 10^{23} = 5.18 \times 10^{23}$ atoms.

(d) 1 mole sodium chloride (NaCI) has 1 mole chloride ions.

Thus 6.0 moles of sodium chloride contains $6.0 \times 6.022 \times 10^{23} = 36.132 \times 10^{23}$

This can also be written as 3.61×10^{24} chloride ions.

(e) 1 mole calcium chloride ($CaCl_2$) has 2 moles of chloride ions

Thus 6.0 moles of calcium chloride contains $2 \times 6.0 \times 6.022 \times 10^{23} = 72.264 \times 10^{23} = 7.23 \times 10^{24}$ chloride ions.

2. How many moles are present in each of the following

(a) 93×10^{23} silver atoms
(b) 3.7×10^{26} molecules of ammonia (NH_3).

Solution

(a) We know that there are 6.022×10^{23} silver atoms in 1.00 mole of silver.

Thus there is 1 silver atom present in

$$\frac{1}{1 \times 6.022 \times 10^{23}}$$ moles of silver.

Thus 9.3×10^{23} silver atoms will occur in

$$\frac{1}{1 \times 6\ 022 \times 10^{23}} \times 9.3 \times 10^{23}$$

= 1.54 moles of silver.

(b) We know that there are 6.022×10^{23} ammonia molecules in 1.00 mole of ammonia.

Thus there is 1 ammonia molecule present in

$$\frac{1}{1 \times 6.022 \times l0^{23}}$$ moles of ammonia.

Thus 3.7×10^{26} ammonia molecules will Occur in $\frac{1}{1 \times 6.022 \times l0^{23}} \times 3.7 \times 10^{26}$

= 6.1×10^{2} moles of ammonia.

Mole calculations with equations

A balanced equation tells us the mole ratios of the reactants and products. To see this we will start by looking at the changes in mass when metals undergo combustion. You should have already seen the reaction of magnesium burning in air. It combines with oxygen to form magnesium oxide as shown in the equation,

$2Mg(s) + O_2(g) \rightarrow 2MgO(s)$

This means that:

2 atoms of magnesium react with 1 molecule of oxygen to form 2 formula units of magnesium oxide.

As we have already noted, atoms and molecules are too small for us to measure in the laboratory, so we use moles. We can read this equation as,

2 moles of magnesium react with 1 mole of oxygen to form 2 moles of magnesium oxide.

1 mol Mg = 24.31 g so that 2 mol Mg = 48.62 g
1 mol O_2 = 2 x 16.00 = 32.00 g

1 mol MgO = 24.31 + 16.00 = 40.31 so that 2 mol MgO = 80.62

From the mole ratio in the equation and these mole calculations, we can see that if we burned 48.62 g of magnesium we would need 32.00 g of oxygen and would produce 80.62 g of magnesium oxide.

No matter how much, or how little, magnesium we use, it will always combine with oxygen in the mole ratio shown, 2 mol Mg: 1 mol O_2. Notice that the ratio in the equation does not mean that 2 g of magnesium combines with I g of oxygen to form 2 g of magnesium oxide. An equation tells us the ratio of numbers of particles or moles involved in a reaction, but not the masses.

If we want to work out the amount of a chemical used or produced in a chemical reaction we must:

- change all masses (weights) to moles
- write a balanced equation
- work out the mole ratio from the balanced equation
- change moles back to mass.

<u>Example</u>

How much magnesium oxide would be produced if we burned 5.38 g magnesium?

Solution

- First we convert mass to moles. From the periodic table we know that:

  24.31 g Mg = 1 mol Mg

  Thus 1 g Mg $= \frac{1}{24.31}$ mol Mg

  Thus 5.38 g Mg $= 5\ 38 \times \frac{1}{24\ 31}$
  $= 0\ 221308$ mol Mg

Notice that we do not round off to 2 decimal places at this stage. Use the number in your calculator for the rest of the calculations and only round off at the final answer.

- Next we write our balanced equation to see the mole ratios used and produced when magnesium burns (combustion).
  $2Mg + O_2 \rightarrow 2MgO$
  From this equation we see that:
  2 mol Mg produces 2 mol MgO
  Thus 1 mol Mg produces 1 mol MgO.
  But we only have 0.221308 mol Mg. Using our mole ratios we see that:

0.221308 mol Mg produces 0.221308 mol MgO

- Now we change the number of moles of MgO to grams. When we add the molar masses of the elements from the periodic table, we find the molar mass of MgO:

  1 mol MgO has a mass of 24.31 + 16 = 40.31 g

  Thus 0.221308 mol of MgO would have a mass of 40.31 x 0.221308 = 8.92 g MgO

  Notice that we have reached the end of our calculations so we can now round off.

- Finally, we have found that burning 5.38 g of Mg would produce 8.92 g MgO.

Mole ratios are very important for chemists and chemical engineers. They use mole ratios to calculate the yield of metals expected when ores are smelted. This helps them decide whether or not it will be economic to mine the ore and extract the metal. They can also use mole calculations to ensure there is enough oxygen present in the smelting furnace and to calculate the amount of sulfur dioxide that will be emitted and have to be dealt with. Here is a sample calculation using an ore.

Example

lf 20 kg of copper(l) sulfide is smelted,

(a) what will be the theoretical yield of copper?
(b) how much oxygen will be needed for complete combustion?
(c) if the actual yield of copper is 75% of the theoretical yield, how much copper will be obtained?

Solution

(a) There are three steps involved here:

- First, calculate how many moles of Cu_2S you are smelting.

  1 mole Cu_2S= 159.16 g (from the periodic table 63.55 x 2 + 32.06)

So 20 kg Cu_2S $\frac{m}{M} = \frac{20\ 000}{159.16}$

$= 125.6597135$ moles Cu_2S

Again, remember not to round off at this point, only when you give the final answer.

- Now use the equation to find the moles of copper produced:
  $Cu_2S(s) + O_2(g) \rightarrow 2Cu(s) + SO_2(g)$

1 mole of copper sulfide + 1 mole of oxygen produces 2 moles of copper + 1 mole of sulfur dioxide

We see that 1 mole Cu_2S will produce 2 moles Cu

so 125.6597135 moles Cu_2S will produce
2 x 125.6597135 = 251.319427 moles Cu.

- Next change the number of moles of copper to grams:
  1 mole Cu = 63.55 g (from periodic table)

so

251.319427 moles Cu = 63.55 x 251.319427
= 15971.35 g Cu

or 15.97 kg Cu.

Remember you can now round off the answer.

(b) You are using 125.6597135 moles of Cu2S.
From the equation you can see that:

1 mole of Cu_2S needs 1 mole of O_2 to be smelted, so 125.6597135 moles of Cu_2S needs 125.6597135 moles of O_2.

Next, change moles of oxygen to grams:

1 mole O_2 = 32 grams (from periodic table) so 125.6597135 mol = 32 x 125.6597135 g =
4 021.11 g or 4.021 kg of oxygen used.

(c) 15.97135 kg of copper is the theoretical yield.

The actual yield is 75% of this

75 x 15.97135 = 11.98 kg 100

Limiting reagents

In most of the calculations you will be asked to do, you will be told the amount of one of the chemicals reacting and you can assume that there will be plenty of the other chemical to complete the reaction. For example, if you are told that 5 g of calcium undergoes combustion to produce calcium oxide, you can assume that there is enough oxygen present for the combustion of all of the calcium.

However, if you are told how much calcium and how much oxygen is present, you need to check that they are in the correct mole ratio for the reaction. First you write the equation

$2Ca(s) + O_2(g) \rightarrow 2CaO(s)$

This shows us that 2 moles of Ca reacts with 1 mole of O_2 and forms 2 moles of CaO.

If you start with 2 moles of Ca and 2 moles of O_2, all the calcium will be used up before the oxygen and the reaction will stop because you run out of calcium. The calcium will limit your reaction.

On the other hand, if you start with 3 moles of Ca and 1 mole of O_2, all the oxygen will be used up before all the calcium has reacted. In this case the oxygen will limit your reaction.

The reactant that runs out first, the one that is completely used up, is called the limiting reagent. Whenever quantities of both reactants are known, you must check for a limiting reagent before the problem can be solved.

Example

36.46 g of hydrochloric acid is reacted with 32.69 g of zinc to produce hydrogen and a salt.

(a) Calculate the number of moles, before the reaction, of
(i) zinc
(ii) hydrochloric acid.

(b) Write an equation for this reaction.
(c) Which is the limiting reagent for this reaction'?
(d) Calculate the number of moles of salt produced. (e) Calculate the mass of salt produced.

Solution
(a) (i)65.38 g Zn = 1 mol Zn (from the periodic table)

Thus 1 g Zn = $\frac{1}{65.38}$ mol Zn

and 32.69 g Zn = $\frac{32.69}{65.38}$ = 0.5 mol Zn.

(ii) Also from the periodic table, the molar mass of HCI = 1.008 + 35.45 = 36.458 g HCI.
So 1 g HCI = $\frac{1}{65.38}$ mol HCI

and 36.46 g HCI = $\frac{36.46}{36.458}$ = 1.00 mol HCI.

(b) $Zn(s) + 2HCl(aq) \rightarrow ZnCI_2(aq) + H_2(g)$

(c) From the equation in (b), we see that 1 mol Zn reacts with 2 mol HCI.
We have 2 mol of HCI, but only 0.5 mol Zn, so the Zn will run out first.
Thus Zn is called the limiting reagent.

(d) From the equation we see that:
1 mol Zn produced 1 mol $ZnCI_2$ (the salt)
thus 0.5 mol Zn will produce 0.5 mol $ZnCI_2$.

(e) We have calculated that 0.5 mol of the salt ($ZnCl_2$) will be produced. The molar mass of $ZnCI_2$ is found by:
1 mol $ZnCl_2$ = 65.38 + 2 x 35.45 = 136.28 g
Thus 0.5 mol $ZnCI_2$ has a mass of
0.5 x 136.28 = 68.14g.

Gases and Moles

The French chemist Joseph Gay Lussac (1778-1850) found experimentally that when gases react there is a simple relationship between their volumes. He found that the volume of hydrogen gas that reacts with oxygen gas to form water is always in the ratio of 2:1. This means that 2 litres of hydrogen react with 1 litre of oxygen to form 1 litre of water vapour.

Hydrogen(g) +	oxygen(g) $\rightarrow$	water(g)
2 volumes	1 volume	2 volumes
e.g. 2 litres	1 litre	2 litres

Based on the results of this experiment and other similar experiments using different gases, Gay Lussac developed a law called the law of combining gas volumes.

Gay Lussac's law of combining gas volumes states that the ratio of the volumes of gases involved in a chemical reaction can be expressed as simple whole numbers. At the time that Gay Lussac was developing his law, chemists knew nothing about mole ratios and indeed were just developing ideas about the atom.
An English scientist named John Dalton (1766-1844) had developed a model of the atom as a very small particle that could not be split (Figure 4.15). He was concerned that Gay Lussac's experimental results conflicted with his atomic model.

Dalton expected
1 volume + 1 volume $\rightarrow$ 1 volume
H + O $\rightarrow$ HO

Instead, Gay Lussac found
2 volumes + 1 volume $\rightarrow$ 2 volumes
H H +O $\rightarrow$?

To Dalton this meant that each hydrogen particle would have to join up with 1/2 an oxygen particle. This would be impossible if Dalton's theory about atoms being indivisible (not able to be split) were correct.

In 1811 an Italian physicist, Amadeo Avogadro (1776-1856), came up with a solution (Figure 4.16). He suggested the idea of a molecule that could consist of one or more atoms—the molecule would be able to be split, but not the atom. In the case of hydrogen and oxygen, they would each consist of diatomic molecules, so the reaction would become:

HH + HH + OO $\rightarrow$ HOH + HOH
2 volumes 1 volume 2 volumes

This idea fitted both the experimental results and Dalton's theory of the atom.

Avogadro's hypothesis stated that equal volumes of all gases, measured at the same temperature and pressure, contain equal numbers of particles. This hypothesis has now been accepted as a law. If we put this information together with what we now know about moles, we can say that equal volumes of gases have equal numbers of molecules and thus equal numbers of moles. This means that their volumes vary in the same proportion as the number of moles.

$2H_2(g)$ +	$O_2(g)$	$\rightarrow$	$2H_2O(g)$
2 litres	1 1itre		2 litres
2 moles	1 mole		2 moles

Notice that you can only use volume ratios like this when you are dealing with gases. This does not apply to liquids or solids.

Molar volume

The volume occupied by one mole of a gas is called its molar volume. The volume of a gas varies with both temperature and pressure.

For most calculations you will need to calculate the volume at 100 kPa (1 atmosphere) pressure and either 0°C or 25°C. At a pressure of 100 kPa and a temperature of 0°C, 1 mole of any gas always occupies a volume of 22.71 L. At a pressure of 100 kPa (l atmosphere) and a temperature of 25°C, 1 mole of any gas always occupies a volume of 24.79 L. This is surnmarised in Table 4.13.

At 0°C and 100 kPa, 1 mole of any gas contains 6.022×10^{23} particles and occupies 22.71 L. At 25°C and 100 kPa, 1 mole of any gas contains 6.022×10^{23} particles and occupies 24.79 L. The number of moles present in any sample of a gas can be calculated by dividing the volume of the gas by the molar volume at that temperature.

$$\text{Number of moles of gas} = \frac{\text{volume of gas}}{\text{volume of 1 mole}}$$

Table 4.13 Volumes of 1 mole of a gas

Temperature (^{o}C)	Pressure (kPa)	Volume of 1 mole (L)
0	100	22.71
25	100	24.79

Examples

1. If you have 12.40 L of any gas at 25°C and 100 kPa, how many moles of the gas are present?

Solution

1 mol of gas at 25°C and 100 kPa occupies a volume of V_m = 24.79 L

$$\text{Number of moles} = \frac{V}{V_m} \qquad \frac{12.40}{24.79}$$

$$= 0.50 \text{ moles of gas}$$

2. How much hydrogen would you need to burn in order to produce 50 mL of water vapour?

Solution

$2H_2(g) + O_2(g) \rightarrow 2H_2O(g)$

Because the reactants and products are gases, this equation tells us that:

2 mL of water vapour is produced by 2 mL of hydrogen.

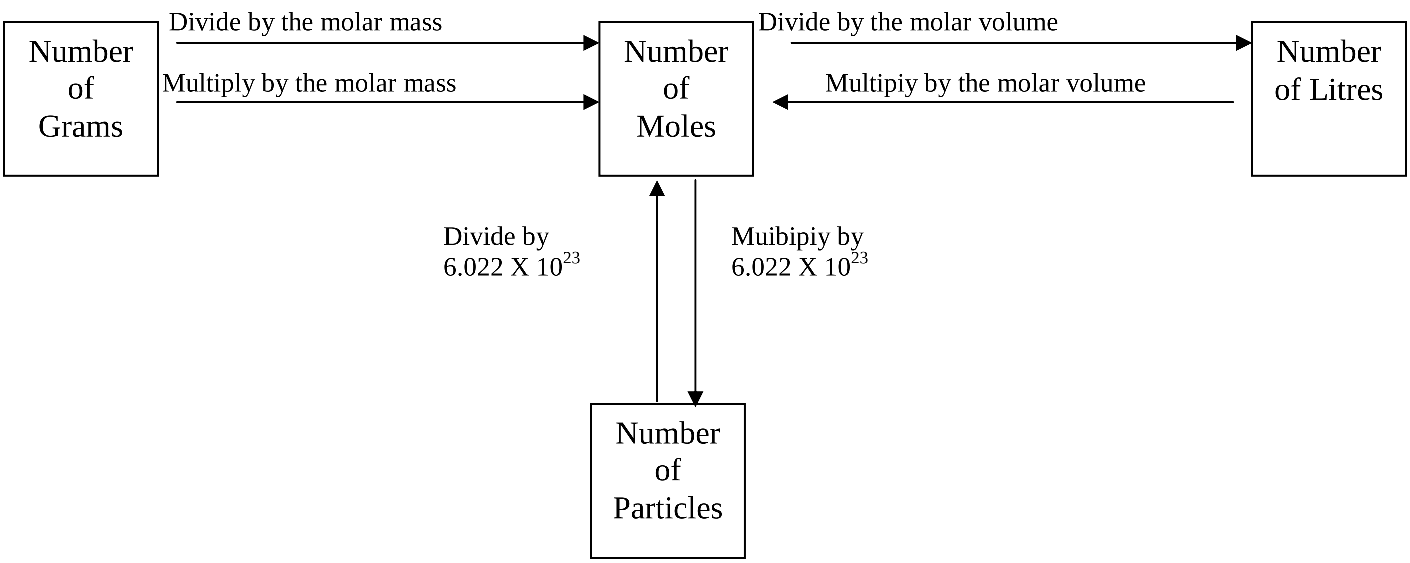
So, 1 mL of water vapour will be produced by 1 mL of hydrogen and 50 mL of water vapour will be produced by 50 mL of hydrogen.

Many of the chemical calculations you will be asked to do start with calculations of how many moles you have or need. Figure 4.17 will help remind you of the relationships between moles and other measurements.

<u>Percentage Composition</u>

The percentage composition of a compound is a relative measure of the mass of each different element present in the compound. We can calculate this either theoretically or practically. To find the theoretical percentage composition, we use atomic mass, as shown in example (a) below. We can find the percentage practically, by decomposing the compound or reacting elements to produce the compound and measuring the amounts of reactants and products, as shown in example (b). This is used to find the percentage composition of ores.

Figure 4.17 Moles The relationship between moles and mass, volume and number of particles



<u>Example</u>

(a) Calculate the theoretical percentage composition of copper(I) sulfide.

(b) If 20 kg of copper(I) sulfide is smelted to produce 12.77kg of copper, what is the experimental percentage composition of the copper sulfide?

(c) Account for the differences in these two answers.

Solution

(a) Formula mass of Cu_2S = 63.55 x 2 + 32.06 = 159.16

$$\text{Percentage of Cu in } Cu_2S = \frac{\text{molar mess of Cu x 100}}{\text{formula mass of } Cu_2S}$$

$$= \frac{127.1}{159.16} \times 100$$

= 79.86% Cu

Composition is 79.86% copper and 20.14% sulfur.

(b) 20 kg of Cu_2S produces 12.77 kg of Cu when smelted. Calculate the percentage composition of Cu_2S.

$$\text{Percentage of Cu in } Cu_2S = \frac{\text{mass of Cu}}{\text{mass of } Cu_2S} \times 100$$

$$= \frac{12.77}{20.0} \times 100$$

$$= 63.85\% \text{ Cu}$$

Composition is 63.85% copper and 36.15% sulfur.

(c) In part (b) the percentage of copper is lower; not all of the copper has been recovered by smelting.

Empirical and molecular formulas

Percentage composition can be used to calculate empirical and molecular formulas of compounds.

The molecular formula shows the actual numbers of atoms of each element in a molecule of the compound. For example, butane has a molecular formula of C_4H_{10}

The empirical formula shows the simplest whole number ratio of the elements present in a compound. For example, the empirical formula of butane is C_2H_5

Example

A hydrocarbon contains 85.4% carbon and 14.6% hydrogen. Its formula mass is 42.08 emu. Find its empirical and molecular formulas.

Solution

- First we find the ratio of carbon atoms to hydrogen atoms:

$$\frac{85.4}{12.01} : \frac{14.6}{1.008}$$

$$= 7.111 : 14.6$$

As in maths we simplify this expression by dividing each number by the smaller number, which in this case is 7.111:

Thus the ratio of carbon atoms to hydrogen atoms:

$$\frac{7.111}{7.111} : \frac{14.6}{7.111}$$

$$= 1 : 2$$

- This tells us that the empirical formula is CH_2.

- We now need to know how many of these CH_2 units there are in a molecule. We can write the molecular formula as C_nH_{2n} and we know the formula mass is 30.

So $(n \times 12) + (2n \times 1) = 42.08$
$14n = 42.08$
$n = 3$
Thus the molecular formula is C_3H_6.