1.21. Formulae, equations and amounts of substance

The mole is the key concept for chemical calculations

DEFINITION: **The mole** is the amount of substance in grams that has the same number of particles as there are atoms in 12 grams of carbon-12.

DEFINITION: **Relative atomic mass** is the **average mass** of one atom compared to one twelfth of the mass of one atom of carbon-12

DEFINITION: **Molar Mass** is the mass in grams of 1 mole of a substance and is given the unit of g mol^{-1}

Molar Mass for a compound can be calculated by adding up the mass numbers(from the periodic table) of each element in the compound
eg $CaCO_3$ = 40.1 + 12.0 +16.0 x3 = 100.1

Calculating amount in moles

$$\textbf{amount} = \frac{\textbf{mass}}{\textbf{MolarMass}}$$

Unit of Mass: grams
Unit of amount : mol

Example 1: Calculate the amount, in mol, in 35g of $CuSO_4$

amount = mass/*M*r

= 35/ (63.5 + 32 +16 x4)

= 0.219 mol

Many questions will involve changes of units
1000 mg =1g
1000 g =1 kg
1000 kg = 1 tonne

1.1) Calculate the amount in mol in 25.0g of $ZnCO_3$?

1.2) Calculate the amount in mol in 30.0g of O_2?

1.3) Calculate the amount in mol in 40.0g of H_2SO_4?

1.4)What is the mass of 0.500 mol of CaF_2?

1.5) What is the mass of 0.250 mol of Li_2CO_3?

1.6) What is the mass of 3.00 mol of $KHSO_4$?

1.7) 0.500 mol of an element weigh 12.15g. What is the relative atomic mass of the element and what is the element?

Example 2: Calculate the number of moles in 75.0mg of $CaSO_4.2H_2O$

moles = mass/*M*r

= 0.075/ (40 + 32.0 +16.0 x4 + 18.0x2)

= 4.36×10^{-4} mol

Avogadro's Constant

The mole is the amount of substance in grams that has the same number of particles as there are atoms in 12 grams of carbon-12.

<u>Avogadro's Constant</u>
There are 6.02×10^{23} atoms in 12 grams of carbon-12. Therefore explained in simpler terms 'One mole of any specified entity contains 6.02×10^{23} of that entity':

Avogadro's Constant can be used for atoms, molecules and ions

1 mole of copper atoms will contain 6.02×10^{23} atoms
1 mole of carbon dioxide molecules will contain 6.02×10^{23} molecules
1 mole of sodium ions will contain 6.02×10^{23} ions

No of particles = amount of substance (in mol) X Avogadro's constant

Example 3: How many atoms of Tin are there in a 6.00 g sample of Tin metal?

amount = mass/Ar

= 6/ 118.7

= 0.05055 mol

Number atoms = amount x 6.02 x 10^{23}

= 0.05055 x 6.02 x 10^{23}

= 3.04 x10^{22}

Example 4: How many chloride ions are there in a 25.0 cm^3 of a solution of magnesium chloride of concentration 0.400 $moldm^{-3}$?

amount= concentration x Volume

$MgCl_2$ = 0.400 x **0.025**

= 0.0100 mol

Amount of chloride ions = 0.0100 x2

= 0.0200

There are two moles of chloride ions for every one mole of $MgCl_2$

Number ions of Cl^- = amount x 6.02 x 10^{23}

= 0.0200 x 6.02 x 10^{23}

= 1.204 x10^{22}

Calculations using the Avogadro constant

In the following questions use this value of the Avogadro constant = 6.0225 x 10^{23}

2.1) How many grams are there in 8.20 x 10^{24} molecules of H_2SO_4?

2.2) How many moles are present in 2.45 x 10^{23} molecules of C_2H_4?

2.3) How many calcium ions are there in 261 grams of $Ca(NO_3)_2$?

2.4) How many grams are there in 2.40 x 10^{24} molecules of NH_3?

2.5) How many grams are there in 6.90 x 10^{25} molecules of H_2?

2.6) How many molecules are there in 0.180 kg of CO_2?

2.7) The mass of one proton is 1.6725 x 10^{-24} g. Calculate the mass of one mole of $^{1}H^{+}$ ions using the Avogadro constant

2.8) The mass of one atom of ^{12}C is 1.99 x 10^{-23}g. Use this information to calculate a value for the Avogadro constant.

2.9) The mass of one mole of ^{1}H atoms is 1.0078g and that of one 1H atom is 1.6734 x 10^{-24}g.
Use these data to calculate a value for the Avogadro constant accurate to five significant figures.

2.10) How does the number of atoms in one mole of helium compare with the number of molecules in one mole of ammonia?

2.11) Calculate the number of moles, and hence the number of molecules, of NH_3 in 0.654 g of ammonia gas.

2.12) Calculate the mass, in grams, of a single atom of sodium (23.0).

2.13) Calculate the number of **atoms** in 1 mol of carbon dioxide

2.14) How many sulfur atoms are there in 0.0350 mol of sulfur S_8 molecules?

2.15) Calculate the number of oxygen **molecules** that react with 2.61 g of sodium.

2.16) 26.2 g of aluminium sulfate, $Al_2(SO_4)_3$, was dissolved in water. Calculate the number of sulfate ions, SO_4^{2-}, present in the solution formed.

Empirical Formula

Definition: An empirical formula is the **simplest** ratio of atoms of each **element** in the compound.

General method

Step 1 : Divide each mass (or % mass) by the atomic mass of the element

Step 2 : For each of the answers from step 1 divide by the smallest one of those numbers.

Step 3: sometimes the numbers calculated in step 2 will need to be multiplied up to give whole numbers.

These whole numbers will be the empirical formula.

The same method can be used for the following types of data:

1. masses of each element in the compound

2. percentage mass of each element in the compound

Example 4 : Calculate the empirical formula for a compound that contains 1.82g of K, 5.93g of I and 2.24g of O

Step1: Divide each mass by the atomic mass of the element

K = 1.82 / 39.1 = 0.0465 mol   I = 5.93/126.9 = 0.0467mol   O = 2.24/16 = 0.14 mol

Step 2 For each of the answers from step 1 divide by the smallest one of those numbers.

K = 0.0465/0.0465 =1   I = 0.0467/0.0465 = 1   O = 0.14 / 0.0465 = 3

Empirical formula =KIO_3

Molecular formula from empirical formula

Definition: A molecular formula is the **actual** number of atoms of each element in the compound.

From the relative molecular mass (*M*r) work out how many times the mass of the empirical formula fits into the *M*r.

Example 5: work out the molecular formula for the compound with an empirical formula of C_3H_6O and a M_r of 116

C_3H_6O has a mass of 58

The empirical formula fits twice into M_r of 116

So molecular formula is $C_6H_{12}O_2$

The *M*r does not need to be exact to turn an empirical formula into the molecular formula because the molecular formula will be a whole number multiple of the empirical formula

Empirical and Molecular formulae questions

3.1) A compound of calcium contains by mass 23.29% of calcium, 18.64% of sulfur and 2.32% of hydrogen, the remainder being oxygen. Determine the empirical formula of this compound.

3.2) Compound **A**, which contains carbon, hydrogen and oxygen only, has 38.7% carbon and 9.68% hydrogen by mass, the remainder being oxygen. Calculate the empirical formula of **A**.

3.3) A chromium compound contains 28.4% of sodium and 32.1% of chromium by mass, the remainder being oxygen. Calculate the empirical formula of this compound.

3.4) A compound **B** contains 36.5% of sodium and 25.5% of sulfur by mass, the rest being oxygen. Calculate the empirical formula of this compound B

3.5) A salt, **C**, contains 16.2% by mass of magnesium, 18.9% by mass of nitrogen and 64.9% by mass of oxygen. Calculate the empirical formula of this compound C

3.6) Compound **D** contains 45.9 % of potassium and 16.5 % of nitrogen by mass, the remainder being oxygen. Calculate the empirical formula of this compound D

3.7) Compound E contains 21.6 % by mass of sodium, 33.3 % by mass of chlorine and 45.1 % by mass of oxygen. Calculate the empirical formula of this compound E

3.8) Analysis of a compound **F** showed that it contained 49.31% of carbon, 6.85% of hydrogen and 43.84% of oxygen by mass. The *M*r of **F** is 146.0. Calculate the empirical formula of **F** and hence deduce its molecular formula.

3.9) Compound G contains 15.38% of carbon, 7.69% of hydrogen, 35.90% of nitrogen and 41.03% of oxygen by mass. Calculate the empirical formula of this compound G

3.10) Ethyne can be used to make compound **H** (*M*r = 215.8) which contains 22.24% carbon, 3.71% hydrogen and 74.05% bromine, by mass. Calculate the empirical formula of H and hence deduce its molecular formula.

3.11) Concentrated nitric acid reacts with magnesium to form an oxide of nitrogen which contains 30.4% by mass of nitrogen. Calculate the empirical formula of this oxide of nitrogen.

3.12) An oxide of nitrogen contains 25.9% by mass of nitrogen. Determine the empirical formula of this oxide.

3.13) Sulfamic acid contains 14.42% by mass of nitrogen, 3.09% hydrogen and 33.06% sulfur. The remainder is oxygen. Calculate the empirical formula of this sulfamic acid

Combustion Analysis

0.328 g of a compound containing C,H and O was burnt completely in excess oxygen, producing 0.880 g of carbon dioxide and 0.216 g of water. Use these data to calculate the empirical formula of the compound.

Work out moles of CO_2 = Mass of CO_2/*M*r of CO_2
= 0.88/44
=0.02mol

Moles of C in compound = moles of CO_2
= 0.02 mol
→ Mass of C in compound = mol of C x 12
=0.02 x12
=0.24g

Work out moles of H_2O = Mass of H_2O /*M*r of H_2O
= 0.216/18
=0.012mol

Moles of H in compound = 2 x moles of H_2O
= 0.024 mol
→ Mass of H in compound = mol of H x 1
=0.024 x1
=0.024g

Work out mass of O in compound = mass of compound – mass of C – mass of H
= 0.328 – 0.24 -0.024
=0.064

Work out moles of O in compound = Mass of O /*A*r of O
= 0.064/16
= mol 0.004

Work out molar ratio of 3 elements (divide by smallest moles)

C = 0.02/0.004
=5

H = 0.024/0.004
=6

O = 0.004/0.004
= 1

empirical formula = C_5H_6O

Questions

4.1 An Alcohol **X** is analysed by complete combustion.
When 0.500 g of the alcohol **X** is combusted, 1.25 g of carbon dioxide and 0.614 g of water are produced.
Calculate the empirical formula of the alcohol **X**.

4.2 Compound **Y** is a compound containing carbon, hydrogen and oxygen only.
Complete combustion of 3.42 g of compound **Y** produces 5.94 g of carbon dioxide and 3.24 g of water. The relative molecular mass of compound **Y** is 76.0.
Calculate the molecular formula of **Y.**

Hydrated salt

A Hydrated salt contains water of crystallisation

$Cu(NO_3)_2 \cdot 6H_2O$

hydrated copper (II) nitrate(V).

$Cu(NO_3)_2$

Anhydrous copper (II) nitrate(V).

Example 6

$Na_2SO_4 . xH_2O$ has a molar mass of 322.1, Calculate the value of x

Molar mass xH_2O = 322.1 – (23x2 + 32.1 + 16x4)

= 180

X = 180/18

=10

Heating in a crucible

This method could be used for measuring mass loss in various thermal decomposition reactions and also for mass gain when reacting magnesium in oxygen.

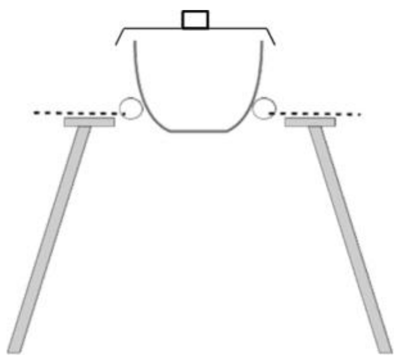
The water of crystallisation in calcium sulfate crystals can be removed as water vapour by heating as shown in the following equation.

$CaSO_4.xH_2O(s) \rightarrow CaSO_4(s) + xH_2O(g)$

Method.

•Weigh an empty clean dry crucible and lid .
•Add 2g of hydrated calcium sulfate to the crucible and weigh again
•Heat strongly with a Bunsen for a couple of minutes
•Allow to cool
•Weigh the crucible and contents again
•Heat crucible again and reweigh until you reach a constant mass (do this to ensure reaction is complete).

The lid improves the accuracy of the experiment as it prevents loss of solid from the crucible but should be loose fitting to allow gas to escape.



Large amounts of hydrated calcium sulfate, such as 50g, should not be used in this experiment as the decomposition is like to be incomplete.

Small amounts the solid , such as 0.100 g, should **not** be used in this experiment as errors in weighing are too high.

The crucible needs to be dry otherwise a wet crucible would give an inaccurate result. It would cause mass loss to be too large as water would be lost when heating.

Example 7 3.51 g of hydrated zinc sulfate were heated and 1.97 g of anhydrous zinc sulphate were obtained.
Use these data to calculate the value of the integer *x* in $ZnSO_4.xH_2O$

Calculate the mass of H_2O = 3.51 – 1.97 = 1.54g

Calculate moles of $ZnSO_4$ $= \frac{1.97}{161.5}$ = 0.0122

Calculate moles of H_2O $= \frac{1.54}{18}$ =0.085

Calculate ratio of mole of $ZnSO_4$ to H_2O $= \frac{0.0122}{0.0122}$ =1 $= \frac{0.085}{0.0122}$ =7

X = 7

Questions on hydrated salts

5.1) In an experiment, the *Mr* of a different hydrated sodium carbonate was found to be 250. Use this value to calculate the number of molecules of water of crystallisation, *x*, in this hydrated sodium carbonate, $Na_2CO_3.xH_2O$

5.2) Hydrated sodium carbonate has the formula $Na_2CO_3.10H_2O$. Calculate the percentage, by mass, of Na_2CO_3 in hydrated sodium carbonate.

5.3) A hydrated sodium sulfate contains 44.1% by mass of sodium sulfate. Hydrated sodium sulfate can be represented by the formula $Na_2SO_4.\ xH_2O$ where *x* is an integer. Calculate the value of *x*.

5.4) Hydrated calcium nitrate can be represented by the formula $Ca(NO_3)_2.xH_2O$ where *x* is an integer. A 9.06 g sample of $Ca(NO_3)_2.xH_2O$ contains 2.76 g of water of crystallisation. Use this information to calculate a value for *x*.

5.5) 6.57 g of hydrated zinc sulfate ($ZnSO_4.xH_2O$) was heated and 3.69 g of anhydrous zinc sulfate was obtained . Use this information to calculate the value of the integer *x* in $ZnSO_4.xH_2O$

5.6) If 15.82g of hydrated sodium thiosulfate $Na_2S_2O_3.5H_2O$ are heated to remove the water of crystallisation, what is the maximum mass of anhydrous sodium thiosulfate that will form?

Answers

1.1) 0.199mol
1.2) 0.9375mol
1.3)0.408mol
1.4)39.1g
1.5) 18.5g
1.6) 408.6g
1.7) 24.3 Mg

2.1)1336g
2.2) 0.407mol
2.3) 9.58×10^{23}
2.4) 67.7g
2.5) 229g
2.6) 2.46×10^{24}
2.7)1.0073g
2.8) 6.03×10^{23}
2.9) 6.0225×10^{23}
2.10) the same
2.11) 2.32×10^{22}
2.12) 3.82×10^{-23}
2.13) 1.81×10^{24}
2.14) 1.69×10^{23}
2.15) 1.71×10^{22}
2.16) 1.38×10^{23}

3.1) $CaSH_4O_6$
3.2) CH_3O
3.3) Na_2CrO_4
3.4) Na_2SO_3
3.5) MgN_2O_6
3.6) KNO_2
3.7) $NaClO_3$
3.8) $C_3H_5O_2$ and $C_6H_{10}O_4$
3.9) $CH_6N_2O_2$
3.10) C_2H_4Br and $C_4H_8Br_2$
3.11) NO_2
3.12) N_2O_5
3.13) H_3NSO_3

4.1) $C_5H_{12}O$
4.2) $C_3H_8O_2$

5.1) 8
5.2) 37%
5.3) 10
5.4) 4
5.5) 7
5.6) 10.08g