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

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

Unit of Mass: grams
Unit of amount : mol

Example 1: What is the amount, in mol, in 35g of $CuSO_4$?

amount = mass/Mr

= 35/ (63.5 + 32 +16 x4)

= 0.219 mol

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?

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.

Avogadro's Constant
There are 6.02 x 10^{23} atoms in 12 grams of carbon-12. Therefore explained in simpler terms 'One mole of any specified entity contains 6.02 x 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 x 10^{23} atoms
1 mole of carbon dioxide molecules will contain 6.02 x 10^{23} molecules
1 mole of sodium ions will contain 6.02 x 10^{23} ions

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

Example 2: 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 6.02×10^{23}

= $0.05055 \times 6.02 \times 10^{23}$

= 3.04×10^{22}

Example 3: 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 6.02×10^{23}

= $0.0200 \times 6.02 \times 10^{23}$

= 1.204×10^{22}

Calculations using the Avogadro constant

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

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

2.2) How many moles are present in 2.45×10^{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 2.40×10^{24} molecules of NH_3?

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

2.6) How many molecules are there in 180 grams of CO_2?

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

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

2.9) The mass of one mole of ^1H atoms is 1.0078g and that of one 1H atom is 1.6734×10^{-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 sulphur atoms are there in 0.0350 mol of sulphur 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 I = 5.93/126.9 O = 2.24/16

= 0.0465 mol = 0.0467mol = 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 I = 0.0467/0.0465 O = 0.14 / 0.0465

=1 = 1 = 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 (Mr) work out how many times the mass of the empirical formula fits into the Mr.

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 Mr 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 sulphur 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 sulphur 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

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 sulphate crystals can be removed as water vapour by heating as shown in the following equation.

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

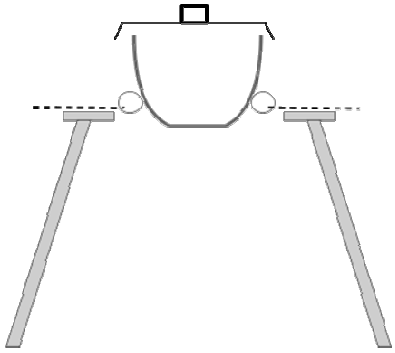
Method.

- Weigh an empty clean dry crucible and lid .
- Add 2g of hydrated calcium sulphate 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).

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

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.

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.



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

Example 7 3.51 g of hydrated zinc sulphate 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

4.1) In an experiment, the *M*r 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, $Na_2CO_3.xH_2O$

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

4.3) A hydrated sodium sulphate 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*.

4.4) 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*.

4.5) 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 $ZnSO_4.xH_2O$

4.6) If 15.82g of hydrated sodium thiosulphate $Na_2S_2O_3.5H_2O$ are heated to remove the water of crystallisation, what is the maximum mass of anhydrous sodium thiosulphate 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}

3.1) $CaSH_4O_8$
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) 8
4.2) 37%
4.3) 10
4.4) 4
4.5) 7
4.6) 10.8g