AS Level calculations involving solids (A First Year Blog)

- You have to be able to deal with all these types of calculations for 'AS' Level Chemistry.

- You may have learnt a bit about calculations involving Mass at GCSE Level, but even so let me remind you about some of the different types of calculations involving Mass. I will start with the most basic type of calculations to provide RMM and RFM from RAM, and I will then go on and cover the following types of calculation.

Section

A) **Calculations using RAM to find RMM and RFM**
B) **Calculations involving moles of ions**
C) **Composition by Mass**
D) **If so much of one substance, then how much of another?**
E) **What is X?**
F) **What is the Empirical and/or the Molecular Formula?**
G) **Calculation of Yield and Atom Efficiency/Economy**
H) **Limiting and Excess Reactants**

NB It is most unlikely that you will ever be asked to calculate the mass of 1 atom/or 1 molecule/or 1 ionic unit of a substance – and if you are asked to calculate the mass of a substance, then you are almost certainly going to be asked to do so for 1 mole (or a number of moles) of the substance. However, sometimes the examiners can be a bit crafty and ask you to calculate the number of tonnes of something.

A) Calculations using RAM to find RMM and RFM

- Let us start with a very simple calculation. For example,

Q)1 **What is the mass of 1 mole of Water molecules?**

A) The Mass of 1 mole of H_2O molecules = [(2 x RAM of H) + (1 x RAM of O)]g
= [(2 x 1.0) + (1 x 16.0)]g = **18.0g**.

NB1 mole has a mass of 18.0g, therefore this answer is in the g mol^{-1} form.

- OK, let us now do some more complicated calculations. For example, let us do the calculations for the mass of 1 mole of NaCl/Na_2CO_3/H_2SO_4/and $(NH_4)_2SO_4$.

  If you use the theory that we have learnt and your Periodic Table and you will see that

- The Mass of 1 mole of NaCl = (1 x RAM of Na)g + (1 x RAM of Cl)g
  = (1 x 23.0)g + (1 x 35.5)g = **58.5g**.

- The Mass of 1 mole of Na_2CO_3 is = [(2 x RAM of Na) + (1 x RAM of C) + (3 x RAM of O)]g
  = (2 x 23.0)g + (1 x 12.0)g + (3 x 16.0)g = **106.0g**

- The Mass of 1 mole of H_2SO_4 = [(2 x RAM of H) + (1 x RAM of S) + (4 x RAM of O)]g
  = (2 x 1.0)g + (1 x 32.1)g + (4 x 16.0)g = **98.1g**

- The Mass of 1 mole of $(NH_4)_2SO_4$ = **2[**(1x14.0)g + (4x1.0)g**]** + (1x32.1)g + (4x16.0)g
  = **2[**14.0g + 4.0g**]** + 32.1g + 64.0g = **132.1g**

- Now let us do what looks as though it is a more difficult calculation, but which in fact is not any more difficult at all. Do not let the 10 molecules of Water perturb you. [The Water here is not physically wet water like rain, but instead it is a "dry" form of water which is an integral chemical part of an ionic substance that is called a "hydrated" crystal. This water is thus often referred to as the "Water of Crystallisation".]

- The Mass of 1 mole of $Na_2B_4O_7.10H_2O$
  = (2 x 23.0)g + (4 x 10.8)g + (7 x 16.0)g + **10[**(2 x 1.0)g + (1 x 16.0)g**]**
  = 46.0g + 43.2g + 112.0g + 10[2.0g + 16.0g]
  = 46.0g + 43.2g + 112.0g + 10[18.0g]
  = 381.2g

- This calculation is not difficult so long as you remember the "Maths for Chemistry" rules.
  1) Do everything in brackets first.
  2) Do Multiplication and Division next.
  3) Then do Addition and Subtraction.

B) Calculations involving moles of ions

- The calculation of the number of ions in a given mass can sometimes throw students. There is no reason why it should do so – and you will not be thrown if you use your brains. Let us do an example, and you will then see how easy the calculation can be.

Q) How many ions are there in 18.5g of $CaCl_2$?
A) 1 ionic unit of $CaCl_2$ contains (a) two Cl^- ions[1] and (b) one Ca^{2+} ion, therefore there are **3 ions** in one **ionic unit** of $CaCl_2$.
- There are roughly 6.02×10^{23} **ionic units** of $CaCl_2$ in 1 mole of Calcium Chloride,[2]
  and (as we have just seen) there are 3 **ions** in every ionic unit of $CaCl_2$, therefore
  there are roughly $(3 \times 6.02 \times 10^{23})$ **ions** in every mole of ionic units of $CaCl_2$.
- The mass of 1 mole of ionic units of $CaCl_2$ = (1 x RAM of Ca)g + (2 x RAM of Cl) g
  = [40.1 + (2 x 35.5)] g = 111.1g
  therefore there are $(3 \times 6.02 \times 10^{23})$ **ions** = 18.06×10^{23} **ions** in 111.1g of $CaCl_2$.
- If there are 18.06×10^{23} ions in 111.1g of $CaCl_2$,
  then there are X ions in 18.5g of $CaCl_2$
  where $X = \dfrac{[18.06 \times 10^{23}]\text{ ions} \times 18.5\text{g}}{111.1\text{g}} \approx 3.01 \times 10^{23}$ ions (to 3 sig. figs.)
  (Where "≈" stands for "is approximately (or roughly) equal to".)
- **Therefore there are c. 3.01×10^{23} ions in 18.5g of $CaCl_2$.**[3]

NB Please go through each step of that calculation again and again until you are absolutely sure that you UNDERSTAND what I did!

C) Composition by Mass, and % Composition by Mass type of question

- One of the easiest calculations that you could be asked to do is a "% composition by mass" calculation. The formula for this calculation is

$$\textbf{\% Composition by Mass} = \frac{\textbf{[Mass that you are asked about x 100]}}{\textbf{Total Mass}}\ \textbf{\%}$$

[1] **NB Here Cl_2 is NOT one molecule, but two Cl^- ions.**
[2] Please remember that there are roughly 6.0×10^{23} units in one mole of ANYTHING/of EVERYTHING!
[3] Please remember that "c." stands for "circa" the Latin word for approximately or roughly or about.

- For example,

Q) What is the % composition by mass of Oxygen in Sulphuric Acid (H_2SO_4)?

A) Since "M = N x RAM ", the Mass of **Oxygen** per mole of H_2SO_4 molecules
Mass of **Oxygen** = [Number of O atoms x RAM of O atoms]g = (4mol x 16.0gmol^{-1}) = 64.0 g

- Similarly, the mass of 1 mole of H_2SO_4 = [(2x1.0) + (1x32.1) + (4x16.0)] g = 98.1 g

- Therefore % composition of O by mass in H_2SO_4 = $\left[\frac{64.0g \times 100}{98.1g}\right]$ % = **65.24 %**

= 65.2 % to 3 sig. figs. (The number of moles is not a part of the determination of the number of sig.figs.)

- You could also do the same calculation for an Ionic substance e.g.

Q) What is the % composition by mass of Calcium in $CaCO_3$?

A) For every mole of $CaCO_3$
Mass of Ca = (1 x RAM of Ca)g = 40.1g
Total Mass of $CaCO_3$ = [(1x40.1) + (1x12.0) + (3x16.0)]g = 100.1 g
Therefore % composition of Ca in $CaCO_3$ = $\left[\frac{40.1g \times 100}{100.1g}\right]$ % = **40.06 %**

= 40.1 % (to 3 sig. figs.)

Q) Calculate the percentage composition by Mass of Silicon and Oxygen in Silicon (IV) Oxide (which is also called "Silica").

A) Silicon (IV) Oxide has the formula SiO_2.
The Molar Mass[4] of SiO_2 = [28.1 + (2 x 16.0)]g = [28.1 + 32.0]g = 60.1g
Therefore % Composition by Mass of Si = [(28.1g ÷ 60.1g) x 100] % = 46.8% ,
and % Composition by Mass of O = [(32.0g ÷ 60.1g) x 100] % = 53.2 % .
[As a check, the two % compositions must add up to 100% – and indeed they do!]

Q) What is the % Composition by Mass of Mg/S/and O in $MgSO_4$?

A) The Molar Mass of $MgSO_4$ = [24.3 + 32.1 + (4 x 16.0)]g = [24.3 + 32.1 + 64.0]g = 120.4g
% Composition by Mass of Mg = [(24.3g ÷ 120.4g) x 100]% = 20.2%
% Composition by Mass of S = [(32.1g ÷ 120.4g) x 100]% = 26.7%
% Composition by Mass of O = [(64.0g ÷ 120.4g) x 100]% = 53.2%
[Check : [20.2 + 26.7 + 53.2]% = 100.1% which would be 100% without the rounding error.]

[4] "Molar Mass" means "the mass of 1 mole of the substance concerned".

Q) Calculate the % Composition by Mass of the Water in Copper Sulphate crystals.

A) Hydrated Copper Sulphate has the formula $CuSO_4.5H_2O$, therefore
The Molar Mass of $CuSO_4.5H_2O$ = [63.5 + 32.1 + (4 x 16.0) + **5**{(2 x 1.0) + 16.0}]g
= [63.5 + 32.1 + 64.0 + 5{18.0}]g
= [63.5 + 32.1 + 64.0 + 90.0]g = 249.6g
% Composition by Mass of $5H_2O$ = [(90.0g ÷ 249.6g) x 100]% = 36.1%

- This next example is an example of one of the most difficult questions that you could be asked with regard to Mass for First Year 'A' Level. The likelihood of the examiners asking you such a difficult question is very small – but, just in case they do, let me take you through the calculation so that you can see that the same principles are involved as in the easier examples. In actual fact, this sum is NOT all that difficult once you see how to do it. The solution to the problem lies in seeing from the Reaction Equation that **X moles** of a Hydrated substance (i.e. one that includes its Waters of Crystallisation) will generate **the same number of moles** of the Anhydrous substance (i.e. one that no longer includes its Waters of Crystallisation). This gives a Mole Reaction Ratio of 1 : 1. The procedure then is to work out the number of moles of the Hydrated and the number of moles of the Anhydrous substances – and these two numbers must equal each other (**because the Mole Reaction Ratio is 1 : 1**). The things that you therefore need to do are
  - Set out the Reaction Equation
  - Derive the Reaction Ratio
  - Calculate the RFM of the substances involved.
  - Calculate the Number of moles of each from the formula "Mass = N x RFM or RMM ".
  - Equate the number of moles.
  - Do the Mathematics involved to get the answer.

Q) On heating 7.38g of $MgSO_4.XH_2O$, 3.78g of Water (i.e. ALL of the Waters of Crystallisation) were driven off. What is the value of "X"?

A) From the wording of the question, we know that the Mass of XH_2O = 3.78g.
Therefore for 1 mole of $MgSO_4.XH_2O$
NB The Mass of the $MgSO_4$ = Total Mass - Mass of the Water = [7.38 - 3.78]g = 3.60g
- RFM of $MgSO_4$ = [24.3 + 32.1 + (4 x 16.0)] = [24.3 + 32.1 + 64.0] = 120.4 g mol^{-1}
- RFM of $MgSO_4.XH_2O$ = [120.4 + 18.0X] g mol^{-1}

- The Reaction Equation for this reaction is

		$MgSO_4.XH_2O(s)$	⟶	$MgSO_4(s)$	+	$XH_2O(g)$
Mass of each	=	7.38g		3.60g		3.78g
RFM of each	=	[120.4 + 18.0X] g mol^{-1}		120.4 g mol^{-1}		not needed

But, Number of moles, N = (Mass ÷ RFM) , therefore using the RFMs above,
No of moles = $\dfrac{7.38g}{(120.4 + 18.0X)\ g\ mol^{-1}}$ and $\dfrac{3.60g}{120.4\ g\ mol^{-1}}$
[The grams cancel each other out and mol^{-1} below the line becomes mol^{+1} above the line, and **now can you see why it is important to use the g mol^{-1} form for RAM in calculations**!]

- The Reaction Ratio is 1 mole of $MgSO_4.XH_2O$ ⟶ 1 mole of $MgSO_4$, i.e. 1 : 1 , therefore
$\dfrac{7.38}{(120.4 + 18.0X)}$ moles = $\dfrac{3.60}{120.4}$ moles
and, by cross-multiplication $\dfrac{[7.38 \times 120.4]}{3.60}$ = [120.4 + 18.0X]
Therefore 246.82 = [120.4 + 18.0X]
Therefore 18.0X = 246.82 - 120.4 = 126.42
Therefore X ≈ 7.0 **(X has to be an integer)**

- **Therefore the formula of the substance is $MgSO_4.7H_2O$.** Please go through this sum again and again and again and again until you are completely happy that you have understood the procedure involved. It is moderately complicated, but it is ***not*** difficult.

This is one of the most important and most often required calculations in Foundation Chemistry.

D) "<u>If so much of one substance, then how much of another?" type of question</u>

- The examiners might start you off with something simple and ask you e.g.

Q) How many moles of KNO_3 are there in 4.04g of KNO_3?

A) No. of moles, N $= \dfrac{M}{RFM} = \dfrac{4.04\text{ g}}{[(1x39.1) + (1x14.0) + (3x16.0)]\text{ g mol}^{-1}} \approx 0.04$ mol

NBPlease note that the grams have cancelled each other out leaving "mol^{-1}" below the line, and "mol^{-1}" below the line is equal to "mol^{+1}" or "mol" above the line. ["mol" is the accepted abbreviation for "moles".]

- They could then make the question slightly more complicated and say

Q) $2KNO_3$ (s) —> $2KNO_2$ (s) + O_2 (g) , and if 4.04g of KNO_3 (s) were used in an experiment based on this equation, then state how many grams of Oxygen would have been produced.

- OK, before showing you how to answer this question, let me point out that **a reaction equation tells you the number moles but NOT THE MASS of each substance that is reacting with the other substances in the reaction**. For example,

For	$2KNO_3$ (s)	—>	$2KNO_2$ (s)	+	O_2 (g) gives a	
Mole Reaction ratio of	2 moles		2 moles		1 mole	**[Equation (A)]**

or for	H_2 (g) + S (s) + $2O_2$ (g) —> H_2SO_4 (l) gives a
Mole Reaction Ratio of	1 1 2 1

or for	Na_xO_y	—>	xNa	+	yO gives a
Mole Reaction Ratio of	1		x		y

- However, even though a Reaction Equation states a **Mole** Reaction Ratio, and does not explicitly state a **Mass** Reaction Ratio, nevertheless you can derive a Mass Reaction Ratio from a Mole Reaction Ratio simply by using the identity **Mass = N x RFM**, [or **RAM**, or **RMM** (whichever is the appropriate one of the three)].

- OK, let us now calculate the masses of the different substances involved.

RFM of KNO_3	=	[(1x39.1) + (1x14.0) + (3x16.0)] g mol^{-1}	=	101.1 g mol^{-1}
M = N x RFM, therefore				
Mass of **2 moles** of KNO_3	=	2 moles x 101.1 g mol^{-1}	=	**202.2g**, and
RMM of O_2	=	(2 x 16.0) g mol^{-1}	=	32.0 g mol^{-1}
therefore Mass of **1 mole** of O_2	=	1 mol x 32.0 g mol^{-1}	=	**32.0g**.

- Equation (A) above is for 2 moles of KNO_3 and for 1 mole of O_2,
and we now know the mass of 2 moles of KNO_3 and the mass of 1 mole of O_2!

- **OK, before I go on and finish answering the question, I am now going to introduce you to a mathematical methodology/technique for deriving a MASS reaction ratio from a MOLE reaction ratio – and the use of this methodology will solve many of the questions involving the calculation of MASS in Chemistry. Please study this methodology very carefully because it will come in useful again and again.** The methodology involves just three lines, and I would advise you always to write out these three lines every single time in your calculations!

Reaction Equation ....
MOLE Reaction Ratio ....
MASS Reaction Ratio .... **from M= N x (RAM or RMM or RFM)**

If you do so, you will make a lot of Mass calculations very easy to do. Right, let us get back to our question, and use the above methodology!

- **Reaction Equation** $2KNO_3$ (s) —> $2KNO_2$ (s) + O_2 (g)
  Mole Reaction Ratio 2 moles 2 moles 1 mole
  Mass Reaction Ratio (from page 5) **202.2g** **not needed** **32.0g**
  [KNO_2 can be ignored because the question does not ask anything about it.]

- The problem then becomes one of resolving the Simple Proportions that are involved i.e.
  If 202.2g of KNO_3 produce 32.0g of O_2
  then 4.04g of KNO_3 will produce X g of O_2
  where $X = \dfrac{32.0g \times 4.04g}{202.2g} \approx$ **0.64g of O_2**

- OK, that might look a bit complicated, but that is only because I have gone through every step in the logic with you. In practice you could do the sum **MUCH more quickly**, so let us do one much more quickly.

Q) H_2 (g) + S (s) + $2O_2$ (g) —> H_2SO_4 (aq) , and if 9.76g of O_2 were used, how many grams of H_2SO_4 would have been produced?

A) You can see straight away (from the number of moles of each substance in the reaction equation) that **TWO** moles of Oxygen will produce **ONE** mole of Sulphuric Acid, therefore the question that you must ask yourself is "what is the mass of the two moles of O_2 and what is the mass of the one mole of H_2SO_4" and that will be the **Mass Reaction Ratio**. OK, let us now do that!

The RMM of O_2	= 2 x 16.0 g mol^{-1}	= 32.0 g mol^{-1}
The RMM of H_2SO_4	= [(2 x 1.0) + (1 x 32.1) + (4 x 16.0)] g mol^{-1}	= 98.1 g mol^{-1}

Reaction Equation	H_2 (g) + S (s) + $2O_2$ (g)	—>	H_2SO_4 (aq)
Mole Reaction Ratio	2 moles		1 mole
Mass Reaction Ratio (M = N x RMM)	2mol x 32.0 g mol^{-1} 64.0g		1mol x 98.1gmol^{-1} 98.1g

- And if 64.0g of O_2 produce 98.1g of H_2SO_4
  then 9.76g of O_2 will produce X g of H_2SO_4
  where $X = \dfrac{98.1\ g \times 9.76g}{64.0g} =$ **14.96g or 15.0g** of H_2SO_4.

- **And, as you can see, once you get the hang of these calculations, they are actually very easy indeed!**

- Up to now, the methodology has allowed us to progress from a Reaction Equation to a **Mole** Reaction Ratio, and thence to a **Mass** Reaction Ratio. However, we are now going to do a type of question where we go from a **MASS** Reaction Ratio to a **MOLE** Reaction Ratio!

E) "What is X?" type of question

Q) Compound X has a % composition by mass 74.2% of Sodium and 25.8% of Oxygen. What is X?

A) We do not know what the Formula of X is, but we do know that it contains Sodium atoms and Oxygen atoms, therefore let us say that it contains X Sodium atoms and Y Oxygen atoms, and now we can write two statements both of which will be true
" Na_xO_y —> xNa + yO ", and **" xNa + yO —> Na_xO_y "** , and we can therefore use either of them for the next bit of the calculation. (NB 100% = 74.2% + 25.8%.)

Reaction Equation	Na_xO_y	—>	xNa	+	yO
Mass Reaction Ratio	100g		74.2g		25.8g
Mole Reaction Ratio ($N = \frac{M}{RAM}$)			$\frac{74.2}{23.0} \approx$ **3.23**		$\frac{25.8}{16.0} \approx$ **1.61**

- 3.23 and 1.61 represent the Mole Reaction Ratios, therefore 3.23 and 1.61 represent the ratio of **moles** of Sodium atoms to **moles** of Oxygen atoms, or the ratio of Sodium **atoms** to Oxygen **atoms** – but it is not possible to have a fraction of an atom, therefore if we divide each number by the smaller of the two numbers, then we will get the smallest WHOLE NUMBER of atoms involved, and we now get the following calculation from start to finish

Reaction Equation	Na_xO_y	—>	xNa	+	yO
Mass Reaction Ratio	100g		74.2g		25.8g
Mole Reaction Ratio ($N = \frac{M}{RAM}$)			$\frac{74.2}{23.0} \approx$ **3.23**		$\frac{25.8}{16.0} \approx$ **1.61**
Dividing across by 1.61			2		1

Therefore x = 2, and y = 1, therefore Na_xO_y = **Na_2O** (Disodium Monoxide),
commonly known as **Sodium(I) Oxide**.

- Let's do another one, and you will get the hang of it.

Q) Compound X has a % composition by mass of 2.0% Hydrogen, 32.7% Sulphur, and 65.2% Oxygen. What is X?

If the substance contains 2.0% of H and 32.7% of S and 65.2% of O by Mass,
then 100g of the substance will contain 2.0g of H/32.7g of S/and 65.2g of O, therefore

A)

Reaction equation	$H_xS_yO_z$	—>	xH	+	yS	+	zO
Mass Reaction Ratio	100g		2.0g		32.7g		65.2g
Mole Reaction Ratio ($N = \frac{M}{RAM}$)			$\frac{2.0}{1.0} =$ **2.0**		$\frac{32.7}{32.1} \approx$ **1.0**		$\frac{65.2}{16.0} \approx$ **4.1**
Which to the nearest whole numbers =			2		1		4

Therefore x = 2, and y = 1, and z = 4 therefore $H_xS_yO_z$ = **H_2SO_4** (Sulphuric Acid).

- The examiners sometimes vary this question by asking

Q) If 127g of Cu react with Oxygen to produce 143g of Copper Oxide, then which Copper Oxide has been formed?

A) Since only Copper and Oxygen are involved, the first fact that we can deduce is that the Conservation of Mass Law requires that (143g-127g =) 16g of Oxygen were involved in this reaction.

Reaction Equation	xCu	+	yO	—>	Cu_xO_y
Mass Reaction Ratio	127g		16g		143g
Mole Reaction Ratio ($N = \frac{M}{RFM}$)	$\frac{127}{63.5} \approx 2.0$		$\frac{16}{16} = 1.0$		

Therefore x = 2, and y = 1 , therefore Cu_xO_y = Cu_2O (Cuprous Oxide, or Copper(I) Oxide).

- As it happens, Oxygen has a diatomic molecule, therefore the correct Reaction Equation would have been **$4Cu + O_2 \longrightarrow 2Cu_2O$**, but that does not alter the **mathematics** of our calculations. The ratio of 2 Cu atoms to 1 O atom will be the same. However, please do not take my word for it. Redo the calculation but this time use the Reaction Equation $xCu + yO_2 \longrightarrow Cu_xO_{2y}$ and see whether you get a different answer!

Reaction Equation	xCu	+	yO_2	$\longrightarrow$	Cu_xO_{2y}
Mass Reaction Ratio	127g		16g		143g
Mole Reaction Ratio $(N = \frac{M}{RFM})$	$\frac{127}{63.5} \approx 2.0$		$\frac{16}{32} = 0.5$		

Now divide across by the smallest number (0.5) and you get x = 4, and y = 1 , which gives $2Cu_2O$ (Cuprous Oxide, or Copper(I) Oxide).

- Sometimes dividing by the smallest number does not give the whole numbers of atoms that are required, and then the resultant decimal numbers must be multiplied to achieve the required whole number of atoms. Let us try one of these.

Q) Given that 0.72g of Mg reacted with 0.28g of Nitrogen, what was the formula of the resultant product?

A)

Reaction equation	xMg	+	yN	$\longrightarrow$	Mg_xN_y
Mass Reaction Ratio	0.72g		0.28g		1.00g
Mole Reaction Ratio $(N = \frac{M}{RFM})$	$\frac{0.72}{24.3} \approx 0.03$		$\frac{0.28}{14.0} \approx 0.02$		

- "0.03" and "0.02" represent the number of moles or the number of atoms of Mg and N which react with each other to form Mg_xN_y, but it is not possible to have a non-whole number of atoms, therefore the technique now is
  a) to divide both these numbers by the smallest number in the group – and this should then convert all the numbers into whole numbers. [In this instance, dividing by 0.02 gives 1 and 1.5, therefore step 2 is
  b) then to multiply the resulting numbers by the *smallest* number that is necessary to achieve a set of whole numbers (here that number will be "2"), and we now get the following calculation from start to finish

Reaction equation	xMg	+	yN	$\longrightarrow$	Mg_xN_y
Mass Reaction Ratio	0.72g		0.28g		1.00g
Mole Reaction Ratio $(N = \frac{M}{RFM})$	$\frac{0.72}{24.3} \approx 0.03$		$\frac{0.28}{14.0} \approx 0.02$		
Divide by smallest number (= 0.02)	1.5		1.0		
Multiply by 2	3		2		

Therefore x = 3, and y = 2 , therefore $Mg_xN_y = Mg_3N_2$ [Magnesium(II) Nitride]

- However, if you had started with "N_2" you would have got the answer in one go.

Reaction equation	xMg	+	yN_2	$\longrightarrow$	Mg_xN_{2y}
Mass Reaction Ratio	0.72g		0.28g		1.00g
Mole Reaction Ratio $(N = \frac{M}{RFM})$	$\frac{0.72}{24.3} \approx 0.03$		$\frac{0.28}{28.0} \approx 0.01$		
Divide by smallest number (= 0.02)	3		1		

Therefore x = 3, and y = 1 , therefore $Mg_xN_{2y} = Mg_3N_2$ [Magnesium(II) Nitride]

F) "What is the EMPIRICAL Formula?" and "What is the MOLECULAR Formula?" type of question

NB In order to answer this sort of question you will need to know that an **Empirical** Formula states the **minimum** number of atoms of each element in a substance which together express the formula of a substance, whereas a **Molecular** Formula states the **actual** number of atoms of each element in the substance e.g. the substance that has the Molecular Formula C_4H_{10} will have an Empirical Formula of C_2H_5. [You may already have learnt this at GCSE Level – and if so I put it in here merely to remind you of the fact.]

Q If 12g of Carbon reacted completely with 2g of Hydrogen to form a substance with an RMM of 56, then what is the Empirical Formula and what is the Molecular Formula of the substance?

Answer

Ai) The Conservation of Mass Law tells us that 14g of the substance must have been produced, and in order to find out the substance produced, we need to start with a Reaction Equation viz

Reaction Equation	xC	+	yH	—>	C_xH_y
Mass Reaction Ratio	12g		2g		14g
Mole Reaction Ratio ($N = \frac{M}{RAM}$)	$\frac{12}{12} = 1$		$\frac{2}{1} = 2$		

Therefore x = 1, and y = 2 , therefore **the Empirical Formula of the substance formed was CH_2.**

Aii) The substance had an RMM of 56, but the RMM of CH_2 = 12 + 2 = 14, therefore there must be **four** lots of CH_2 in the substance (because 4 x 14 = 56), **therefore the substance has a Molecular Formula of C_4H_8.**

- Easy, isn't it!

Q) A compound which has an RMM of 78 contains 92.3% C and 7.7% H by Mass. What is the Empirical Formula and what is the Molecular Formula? Magnesium(II) Nitride

A) If the substance contains 92.3% C and 7.7% H by Mass, then 100g of the substance will contain 92.3g of C and 7.7g of H, and in order to find out the substance produced, we need to start with a Reaction Equation.

Reaction Equation	xC	+	yH	—>	C_xH_y
Mass Reaction Ratio	92.3g		7.7g		100g
Mole Reaction Ratio ($N = \frac{M}{RAM}$)	$\frac{92.3}{12.0} = 7.7$		$\frac{7.7}{1.0} = 7.7$		

Divide by the smallest number to obtain a whole number of atoms, and this gives a ratio of 1 : 1 therefore **the Empirical Formula of the substance is CH.**

- However, the RMM of CH is 13 whereas the RMM of the substance is 78, therefore there must be six lots of CH in the substance (because 6 x 13 = 78).
- **Therefore the Molecular Formula of the substance must be C_6H_6 (viz. Benzene).**

Q) What is the EMPIRICAL Formula of the substance which has a % composition by mass of 82.8% Carbon and 17.2% Hydrogen, and if it has an RMM of 58, what is its Molecular formula?

Answer

A1) **Reaction equation**	C_xH_y	—>	xC	+	yH
Mass Reaction Ratio	100g		82.8g		17.2g
Mole Reaction Ratio ($N = \frac{M}{RAM}$)			$\frac{82.8}{12.0} = \mathbf{6.9}$		$\frac{17.2}{1.0} = \mathbf{17.2}$
Dividing across by 6.9 we get			1.0		2.5

But, we still do not have a whole number of atoms, therefore since there is a half number of atoms in the answer, we must now multiply the answer by 2 to get the smallest **whole** number of atoms

= 2 5

Therefore x = 2, and y = 5, therefore C_xH_y = $\mathbf{C_2H_5}$!

A2) However, the RMM of this substance is [(2 x 12.0) + (5 x 1.0)] = 29.0 and the RMM of the substance in the question is 58, therefore (since 58 = 2 x 29) the Molecular Formula of the substance must have twice as many atoms as the Empirical Formula – therefore the Molecular Formula of the substance in question is **C_4H_{10}**!

- I will do one last example. It is more complicated than the standard question, and you may be set one of these at 'A' Level these days.

Q) 1.00g of a substance that contained nothing but Carbon, Hydrogen and Oxygen was burnt in excess Oxygen to produce 2.52g of CO_2 and 0.443g of H_2O. What is the Empirical Formula of the substance that was burnt?

A) In order to find out the identity of the substance that was burnt, we need to know the Reaction Equation, and in order to do this, we need to know the Mass Reaction Ratio and the Mole Reaction Ratio. Let us calculate the Mass Reaction Ratio first of all.

<u>Mass of C</u>

- All the substance was converted into Carbon Dioxide and Water therefore **the Mass of C in the substance must be the same as the Mass of C in the CO_2**.
- The RMM of CO_2 = [12 + 2x(16)] = 44, and the proportion of C in CO_2 = (12 ÷ 44), therefore
- Mass of C in CO_2 = 2.52g x (12 ÷ 44) = **0.6873g**

<u>Mass of H</u>

- Using the same logic, the Mass of H in the substance must be the same as the Mass of H in the H_2O, and the proportion of H in H_2O = (2 ÷ 18), therefore
- Mass of H in H_2O = 0.443g x (2 ÷ 18) = **0.0492g**

<u>Mass of O</u>

- The substance contained nothing but Carbon, Hydrogen and Oxygen, and since we have ascertained the Mass of the Carbon and the Mass of Hydrogen in the substance, then **the remainder of the Mass of the substance MUST be Oxygen**!

- Therefore Mass of O = [1.00 - (0.6873 + 0.0492)] g = **0.2635g**

- We can now utilise our normal technique

Reaction Equation	xC	+	yH	+	zO	—> $C_xH_yO_z$
Mass Reaction Ratio	0.6873g		0.0492g		0.2635g	
Mole Reaction Ratio ($N = \frac{M}{RAM}$)	$\frac{0.6873}{12.0}$ = 0.0573		$\frac{0.0492}{1.0}$ = 0.0492		$\frac{0.2635}{16.0}$ = 0.0166	
Divide by the smallest number	3.5		3.0		1.0	
but 3.5 is not an integer, therefore we must multiply all of the numbers by 2 to get	7.0		6.0		2.0	

- **Therefore the Empirical Formula of the substance is $C_7H_6O_2$.**

G) <u>The Calculation of Yields</u>

- In Organic Chemistry (Chains & Rings) the yield from a reaction is rarely what it should theoretically be, and it could be say 60% of the theoretical yield.

- The examiners quite often ask you to do a Yield calculation, and this is how you do it.

$$\text{Yield } \% = \left[\frac{\text{Actual Mass of Product obtained}}{\text{Theoretical Mass of Product}} \times 100 \right] \%$$

- Let us do an Organic Chemistry example, and because I have (as yet) not taught you anything about Organic Chemistry, do not worry about the reaction itself.

Q) From the reaction of 10g of 1-Bromobutane with NaOH, 3.9g of Butan-1-ol were obtained. What was the Yield? (We will talk about the conversion of a halogenated alkane into an Alcohol when we get to Organic chemistry.)

A) Reaction Equation	C_4H_9Br	+	NaOH	—>	C_4H_9OH	+	NaBr
Molar Mass	= [(4x12)+(9x1)+80]g		(23+16+1)g		(48+9+16+1)g		(23+80)g
	= 137g		40g		74g		103g

- The answer to the problem now becomes one of simple proportions :
  If 137g of C_4H_9Br generates 74g of C_4H_9OH
  10g of C_4H_9Br generates X of C_4H_9OH
  where $X = \frac{74g \times 10g}{137g} = 5.4g$, therefore the Theoretical Mass = 5.4g.
- But, Actual Mass obtained = 3.9g, therefore
- $\text{Yield \%} = \left[\frac{\text{Actual Mass of Product obtained}}{\text{Theoretical Mass of Product}} \times 100\right]\% = \frac{3.9g \times 100\%}{5.4g}$
- **Yield % = 72.2%**

H) Atom Economy (or Atom Efficiency)

$$\text{Atom Economy} = \frac{\text{Mass produced of the desired product}}{\text{Mass of all the objects produced}}$$

- There are two ways of looking at how much of a desired product is being made/achieved, and we have just examined the first way of doing so viz. it is to compare how much of a product was **actually made** in comparison to how much should **theoretically have been produced**.

- The second comparison that could be made is to ask how much of the desired product was made in comparison to everything that was made.

- In the olden days (before Portland cement was invented in the 1800s), the mortar that was used in holding bricks together (until about 200 years ago) was a lime and sand mixture (where today it is a cement sand mixture). The “lime” that was used was obtained by burning Calcium Carbonate, $CaCO_3$ (usually in the form of chalk or limestone) at a high temperature in a kiln
  $$CaCO_3\,(s) \longrightarrow CaO\,(s) + CO_2\,(g)$$
  and “lime” is still made today using that method (but it is used mainly in rebalancing soils that are too acidic for the purpose of growing certain types of vegetables).

- Let us now do an Atom Economy (or Atom Efficiency) calculation. If 500 kg of CaO are produced when 1,000 kg of $CaCO_3$ are burnt, then what is the Atom Economy?

- The law of the Conservation of Energy says that the mass of the CO2 (g) and the mass of the CaO (s) must be equal to the mass of the $CaCO_3$ (s), therefore
  Mass of the desired product 500 kg, and
  Mass of all the products produced 1,000 kg therefore the

$$\textbf{Atom Economy} = \frac{\mathbf{500\ kg}}{\mathbf{1{,}000\ kg}} = \mathbf{50\%}$$

- The two methods give different answers. The Atom Economy gives a smaller answer than the Yield and indicates that the **efficiency** of the process is not that high.

I) Limiting Reactants and Excess Reactants

Q If 5.0g of Iron were mixed with 5.0g of Sulphur, and the resulting mixture were reacted, how much FeS did it produce, and which substance was the limiting reactant, and which was in excess?

A We know that Fe + S —> FeS, therefore the Reaction Ratio is 1 : 1 , but
this does NOT mean that 5g of Fe react with 5g of S !

- What it does mean is that

  1 MOLE of Fe + 1 MOLE of S —> 1 mole of FeS

- We therefore have to convert the Masses of the substances given into **moles** in order to find out how much of each element reacted with the other. **N = M ÷ RAM**, therefore
  Number of moles of Fe = (Mass of Fe) ÷ (RAM) = 5.0g ÷ 55.9gmol^{-1} = 0.0894 mol
  Number of moles of S = (Mass of S) ÷ (RAM) = 5.0g ÷ 32.1gmol^{-1} = 0.1558 mol

- The Reaction Ratio is 1 : 1, therefore whatever happens
  0.0894 moles of Fe can react with ONLY 0.0894 moles of S out of the 0.1558 moles of S – so **there is too much of S** for the amount of Fe involved. The phrase that Chemists use for this is that S is "**in excess**" and that consequently the reaction is limited by the amount of Fe that is present viz. Fe is the **limiting reactant**! I'll say that again, here **S is "in excess" and Fe is the limiting reactant**!

- This means that (0.1558 - 0.0894 =) 0.0664 moles of S will be unused/unreacted
  (i.e. **it is the amount of S which is in excess of the requirements of this reaction**).

- What we have now established therefore is that
  0.0894 moles of Fe + 0.0894 moles of S —> 0.0894 moles of FeS
  and we can now work out the Mass of the FeS produced.

- **Mass of FeS = Number of moles of FeS x RFM of FeS**
  = 0.0894mol x (55.9 + 32.1) gmol^{-1} = 7.87g of FeS
  and there are 0.0664 moles of S (= 2.13g of S) left over.

- Nice and easy wasn't it! There are many calculations that can be done with regard to Solids, and I would strongly urge you to work through as many calculations involving Solids as you can from Eileen Ramsden's "Calculations for 'A' Level Chemistry", and "Advanced Chemistry Calculations" by I.L.P.A.C. (the ISBN No for it is 0 7195 7506 0), or from Jim Clark's excellent book "Calculations in AS/A Level Chemistry".

- **OK, I think that that should have given you a good feel for calculations involving RAM/RFM/RMM. Please make sure that you are comfortable with all the worked examples in this Section.**

- In this Chapter I have done calculations for nothing but SOLIDS, and in Chapter 39 I will show you how to do the calculations for LIQUIDS, and in Chapter 40 I will show you how to do those for GASES.