A First Year blog on Calculations in Chemistry: Part 1, 23rd February 2019

(This is a **revision** blog. It is merely a *summary* of some of the things that you need to know. *Everything in this blog can be found in Chapters 35-41 of the First Year, Foundation Chemistry Book*.)

You do not have to be Paul Dirac[1] or Andrew Wiles[2], to be able to do the calculations that are involved in 'A' Level Chemistry. You do not even have to be doing 'A' Level Maths – but you do have to be numerate! You must know straightforward things such as the Rule of Simple Proportions and the Rule of the Equality of Treatment, and I would urge you as strongly as I possibly can to read Section 1.3 of "Some Introductory Stuff (Optional)" on this website. The next thing that I would urge you to read is Chapters 35-41 of the First Year, Foundation book. Doing so will not only tell you how to do all the calculations that you will encounter in 'A' Level Chemistry, but it will show you how to do the calculations *in the quickest possible time*. Many students are not able to finish all the questions on the exam paper, not because they do not know the stuff, but because they have not practised doing the calculations involved often enough. If you genuinely want an A or an A* in Chemistry, then you must master the Mathematical bits of Chemistry. Jim Clark's "Calculations in AS / A Level Chemistry" is very good[3], but "Advanced Chemistry Calculations" by Lainchbury, Stephens and Thompson has the advantage for the 'not-so-confident' mathematician in that the authors give, not just the answers, but **the *workings* to every single question that they set in the book**. It really is an admirable book for the mathematical novice.

Where does one start with the Maths of Chemistry?

My answer is that unless you start with what a "mole" is, then you will make your life very difficult indeed. The number that you were given at GCSE Level was 6.0×10^{23}, but I am not sure how far forward one has got by knowing that number. It is such a colossally large number of units that I suspect that there is no human being who can really comprehend such a large number.

$$\mathbf{6.0 \times 10^{23} = 600{,}000{,}000{,}000{,}000{,}000{,}000{,}000}$$

and that is just an *approximation* of Avogadro's Constant. What is more, even if I told you the numerals that follow on from 6.0 are " $\mathbf{6.022{,}140{,}760 \times 10^{23}}$ you would not be any the wiser. Let me make it even more incomprehensible by telling you that in just one 10 ml or 10cm^3 teaspoonful of water there are

334,000,000,000,000,000,000,000 (or $3.342{,}796{,}149 \times 10^{23}$)

and you will then throw up your hands in horror and say "I give up. I will go and do something simple like becoming a neurosurgeon or a rocket scientist or solving the Middle-East crisis"!

Well, luckily you do not have to panic, because it is precisely because of the *incomprehensibility* of such large numbers that the "**mole**" was invented!

However, let me start somewhere else. If you went to a shoe shop and wanted to buy two shoes (a left and a right shoe for yourself) you would ask for a **pair** of shoes (because the unit of counting in shoes is one "pair"), and if you went to Tesco and wanted 12 eggs you would buy one "**dozen**" eggs (because the unit of counting eggs is one "dozen"). Similarly if you went into a shop that sold molecules, you would not ask for 602,214,076,000,000,000,000,000 molecules, but instead you would ask for one "mole" of molecules – because the unit of counting for very small entities in Chemistry is one "**MOLE**".

The unit of counting for very small entities in Chemistry is one "MOLE".

Moles and Avogadro's Constant

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[1] Paul Dirac was one of the greatest Mathematicians that this country has ever produced.

[2] Andrew Wiles and Jocelyn Bell Burnell are quite possibly the two most modest scientists that I have ever heard interviewed, and in their fields they are quite possibly the most distinguished scientists alive. It is a travesty of justice that Wiles has not been given the Nobel Prize, and Jocelyn Bell's Nobel Prize was "stolen" from her by the 'male' establishment that governed science at the time – and my great hero Fred Hoyle was one of the very few men who stood up for her against the establishment.

[3] I am a huge admirer of Jim Clark. He has forgotten more Chemistry in his life than I will ever learn in my lifetime.

There is no way that atoms/molecules/ions/etc can be counted individually without sophisticated machines. In order to be able to count such small entities, you need therefore to gather them together in *very big groups*, and use each group as one of your units of counting – and that is what "moles" are all about. As it happens, scientists have worked out that there are roughly 6 x 10^{23} atoms of Carbon in 12 grams of Carbon-12 (^{12}C), and scientists eventualy decided to utilise this fact for the counting unit in Chemistry – so now let us start talking like scientists.

If you were to ask me what a mole is, then I would say to you that

A mole is the unit of counting in Chemistry and it consists of exactly the same number of Carbon atoms as there are in 12 grams of Carbon-12.

NB Please remember that we do not know exactly how many atoms there are in 12g of Carbon-12, but whatever that number is, then THAT is **exactly** the number of units that there are in one mole of anything. " $6x10^{23}$ " is merely an approximation of that number, and scientists have now agreed that, from the 20th May 2019, the SI unit for Avogadro's Constant will be $6.022,140,760 \times 10^{23}$ mol^{-1}.

(By the way, the term "mol^{-1}" stands for "per mole" or "for every mole".)

Moles

In order to see the usefulness of moles, let us look at the most famous equation in Chemistry i.e. that of Hydrogen and Oxygen reacting together to form Water viz.

$$2H_2 + O_2 \longrightarrow 2H_2O$$ (cf. footnote[4])

and if you look at the equation you will see that it is doing two things i.e.

a) it is stating what the reactants and the products are, and
b) it is specifying the **proportions** in which the reactants react to produce the product or products.

The equation is thus saying that if you react

2 MOLECULES of Hydrogen + 1 MOLECULE of Oxygen you will get 2 MOLECULES of Water

and (as I shall prove to you shortly) it is also saying that if you react

2 MOLES of Hydrogen molecules + 1 MOLE of Oxygen molecules you get 2 MOLES of Water molecules.

We can therefore note that all Chemical/Ionic/and Molecular reaction equations specify the proportions of the reactants and products either in

a) atoms/molecules/ions , or in
b) MOLES of atoms/molecules/ions.

The Amount of a substance

[4] Strictly speaking the equation should be written as a reversible reaction, but let us not worry about that for the moment.

If you have a pair of something then you have two of those things, and if you have a dozen of something then you have twelve of those things, and so on. *A counting unit describes or defines the number or the* ***amount*** *of things involved.*

If you therefore see the word "amount" in Chemistry, then you are being told the NUMBER OF MOLES of the substance!

The number of particles of a substance is called the **AMOUNT , N ,** of the substance, and the Amount of a substance is always measured in moles. I'll say that again.

In Chemistry, the Amount of a substance is the Number of MOLES of that substance.

1 mole of ANYTHING/EVERYTHING always contains *exactly the same number of units*, namely 1 mole of anything always contains *the same number of units as there are atoms of Carbon in 12 g of C-12* viz c. 6×10^{23} units of that thing, therefore

1 mole of Cl atoms contains c. 6×10^{23} **ATOMS** of Chlorine.
1 mole of Cl_2 molecules contains c. 6×10^{23} **MOLECULES** of Chlorine,
and since ONE mole of Chlorine molecules contains TWO moles of Chlorine atoms
1 mole of Cl_2 molecules contains c. **2** x 6×10^{23} ***ATOMS*** of Chlorine,
1 mole of H_2O molecules contains c. 6×10^{23} **MOLECULES** of Water.
1 mole of NaCl ionic units contains c. 6×10^{23} **IONIC UNITS** of Sodium Chloride.
1 mole of $MgCl_2$ ionic units contains c. 6×10^{23} **IONIC UNITS** of Magnesium Chloride
1 mole of H_2SO_4 molecules contains c. 6×10^{23} **MOLECULES** of H_2SO_4.

1 mole of ANYTHING always contains exactly the same number of units of that thing (that being *roughly* 6×10^{23} units of that thing).

The relationship between moles of MOLECULES and moles of ATOMS

1 **molecule** of H_2SO_4 contains 2 **atoms** of H and 1 **atom** of S and 4 **atoms** of O, therefore
1 mole of H_2SO_4 **MOLECULES** contains **2** x 6×10^{23} Hydrogen **ATOMS**
1 mole of H_2SO_4 **MOLECULES** contains **1** x 6×10^{23} Sulphur **ATOMS**
1 mole of H_2SO_4 **MOLECULES** contains **4** x 6×10^{23} Oxygen **ATOMS** , and
in total 1 mole of H_2SO_4 **MOLECULES** contains **7** x 6×10^{23} ***ATOMS*** (but different sorts of atoms).

The relationship between moles of IONIC UNITS and moles of IONS

1 **IONIC UNIT** of $MgCl_2$ contains 1 **ION** of Mg^{2+} and 2 **IONS** of Cl^-, therefore
1 mole of $MgCl_2$ **ionic units** contains 1 x 6×10^{23} Mg^{2+} **IONS**
1 mole of $MgCl_2$ **ionic units** contains 2 x 6×10^{23} Cl^- **IONS** , therefore
in total 1 mole of $MgCl_2$ **ionic units** contains **3** x 6×10^{23} **IONS** (of whatever sort).

You do not need to remember any of these numbers. All that I am doing is pointing out to you the relationships that are involved.

MOLE Reaction Ratios

We have already learnt that a Reaction Equation tells you about the Proportions in which Reactants react with each other to form Products – but, now that we have learnt about moles, we can derive a new piece of information about Reaction Equations! Let us again consider the reaction equation for the formation of Water.

O_2	+	**$2H_2$**	—>	**$2H_2O$**
1 molecule of O_2		**2 molecules of H_2**	—>	**2 molecules of H_2O**

and, provided that we multiply *both* the Left Hand Side (LHS) and the Right Hand Side (RHS) of the reaction equation by the same number (maintaining the equality of treatment), we would get

	2 molecules of O_2	+	**4** molecules of H_2	—>	**4** molecules of H_2O
or	**4** molecules of O_2	+	**8** molecules of H_2	—>	**8** molecules of H_2O
or	**10** molecules of O_2	+	**20** molecules of H_2	—>	**20** molecules of H_2O
or	we could multiply both sides by 'X' and get				
	1X molecules of O_2	+	**2X** molecules of H_2	—>	**2X** molecules of H_2O

and, if X = **(6×10^{23})** , then we would get

1 x **(6×10^{23})** molecules of O_2 + 2 x **(6×10^{23})** molecules of H_2
—> 2 x **(6×10^{23})** molecules of H_2O

However, (6×10^{23}) = 1 mole, therefore the reaction equation now reads

1 MOLE of molecules of O_2 + 2 MOLES of molecules of H_2
—> 2 MOLES of molecules of H_2O

This is rather exciting, because we have used nothing but our brains to prove the statement that *a reaction equation states the proportions of the reactant atoms/ions/molecules that take part in a reaction – and it also states **the proportions of the MOLES of the reactant atoms/ions/ molecules that take part in the reaction**!*

What we did was to use nothing but our brains to advance the amount of knowledge that we had. This process is called "**deduction**" – and as you get older and you start to think for yourselves more (instead of relying on teachers/friends/books/etc), the more that you deduce new truths for yourself, the better will you become as a student and the more intelligently will you be behaving.

*In the exams that you will sit over the next few years, one of the things that examiners will do is to give you some information and then ask you to "**deduce**" some other information from that (and this will be especially true in Advanced Mathematics)!*

A Reaction Equation sets out the Reactants and the Products of a reaction in a balanced equation. Thus for the reaction equations below

(A) **$HCl(aq)$ + $NaOH(aq)$ —> $H_2O(l)$ + $NaCl(aq)$**
(B) **$H_2SO_4(aq)$ + $Mg(OH)_2(aq)$ —> $2H_2O(l)$ + $MgSO_4(aq)$**

in English, Reaction equation (A) is saying
"1 unit of HCl is reacting with 1 unit of NaOH to form 1 unit of H_2O and 1 unit of NaCl"
and Reaction equation (B) is saying
"1 unit of H_2SO_4 is reacting with 1 unit of $Mg(OH)_2$ to form 2 units of H_2O and 1 unit of $MgSO_4$".

In Part 2 of this blog I will take you through the principles involved in doing calculations for the masses of solids/ the volumes and the concentrations of liquids/ and the volumes of gases.