Equation, Formulas, And More……….

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To express the facts pertaining to a chemical composition and or reaction a kind of short hand was developed to do just that. I received a comment from an individual who read my first article. He was asking if I missed anything in the article which, mainly, was written and geared to atomic theory regarding crystal structure in our rocks and minerals.

Well, maybe I did miss something so here in this article I will try to expand on the subject; however, I am leaning toward mineral assay as a focus in some ways as this article does reference the substances that we find in our earth's crust (rocks). The first example that I am going to relate to requires some introduction. I will be referring to Realgar, Orpiment, Mispickel, and something you all know about and that is pyrite.

Realgar is an arsenic sulfide (AsS or AS_4S_4). It is also known as Ruby sulfur.

This mineral is sectile and comes in a number of forms such as in clusters of monoclinic crystals, or in granular, compact or powdered states.

Orpiment is an arsenic sulfide mineral (As_2S_3) as well. This mineral is usually found in volcanic fumaroles. These are also found in low temperature hydrothermal veins and hot springs.

Now mispickel is also known as Arsenopyrite. It is an iron arsenic sulfide (FeAsS).Very dangerous stuff. This mineral is found in high temperature hydrothermal veins. Also may be found in pegmatites as well as in those metamorphic or metasomatic contact zones. Here is a tip: it serves as an indicator of gold bearing reefs.

I do not believe that I need to add a small description of pyrite. Most people can recognize it and know what it is as a mineral, unless you believe in fool's gold. So let's move on to equations and formulas.

Take for example, the following table. When comparing the composition of the compounds, you might notice that there is no simple way to show the proper proportions for each of the minerals. The composition in the following table only shows the proportions as a whole of the sample and does not really relate to the proportions of the compounds. As one scientist may put it, there is no simple law.

	Realgar	Orpiment	Mispickel	Pyrites
Arsenic	71.4	60.9	46.0	-
Sulphur	28.6	39.1	19.6	53.3
Iron	-	-	34.4	46.7
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	100.0	100.0	100.0	100.0

However, if the above example was calculated using the atomic weights of the compounds, one would notice that some form of a simple law becomes apparent. The composition becomes 107, 246, 163, and 120 parts, and this can be tons, pounds, grams, or whatever. Example: pyrite = 120 grams or ton of which sulphur is 64 parts per 120 grams and iron is 56 parts per 120 grams. This could also be tons instead of grams.

	Realgar	Orpiment	Mispickel	Pyrites
Arsenic	75	150	75	-
Sulphur	32	96	32	64
Iron	-	-	56	56
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	107	246	163	120

What is used here is the periodic table. It is the atomic weight for each compound. Consider the orpiment. Arsenic has an atomic weight of 75, however, orpiment has 2 atoms of arsenic (As_2) and 3 atoms of sulphur (S_3) then this translates into As being 150 and S being 96 and combine would make 246. This would be 246 parts by weight. If one read my first article "Chemistry AddendumTo Physical Geology" one would be familiar with the periodic table, its associated element symbol, and the elements atomic weight.

As you may already know, if there is more than one atom of an element present in the molecule then a small number placed behind the element signifies the number of atoms (FeS_2 or Fe_2S_3). Using Fe_2S_3, we have 2 atoms of iron and 3 atoms of sulphur. However, when a group of atoms is enclosed in brackets, $Pb(NO_8)_2$, the figure after the bracket and under the bracket signifies that you would multiply everything within it. $Pb(NO_8)_2$ can therefore be written as PbN_2O_6.

Once in a while it is easier to represent the atoms of a molecule by dividing it into two or more groups. This is done by separating each simple formula by a period (.). Using slaked lime as an example it formula is CaH_2O_2 and as already mentioned may be written as $Ca(HO)_2$. By separating the formula we would write it as $CaO.H_2O$.

This is where it may get a little more interesting. A (+) sign indicates that there are two substance that are separate from each other. Continuing to use calcium oxide and water as our example we would show the two substances as $CaO + H_2O$. Where we have an equal sign (=), it refers to the reaction of combining the two substances, or simply put, the products of the reaction. By combining the two statements we get an equation. In this instance lime and water creates slaked lime.

CaO	+	H_2O	=	CaH_2O
↓		↓		↓
Ca=40		H_2=2=1x2		Ca=40
O=16		O=16		H_2=2=1x2
----		----		O_2=32=16x2
56		18		----
				74

As you may have guessed, if you combine 56 parts of lime with 18 parts of water, you would produce 74 parts of slaked lime. It doesn't really make much sense but consider this; how much lime would it take to produce 112lbs of slaked lime. Well let's see. $56\ X\ 112 \div 74$. We would need about 84¾ lbs. of lime to make 112 lbs. of slaked lime.

Let's look at another example in a similar way. Let's say for this example, that you were in the field, and picked up some nice samples containing tin oxide (SnO_2). You take 5 grams of material and you want to refine it down to just tin (Sn). In order to do this you will need to liberate the oxygen leaving the tin as the element. You would have to use potassium cyanide (KCN) to do this with, carefully mind you. The question is how much of the potassium cyanide are you going to need? Refer to the diagram below:

SnO_2	+	$_2KCN$	=	Sn + $_2KCNO$	
↓		↓			
Sn = 118		K = 39			
O_2 = 32		C = 12			
———		N = 14			
150		———			
		65 X 2 = 130			

So, what we are looking for is the relation between the two substances (tin oxide and potassium cyanide). Since 1 molecule of tin oxide has 150 parts and the 1 molecule of the potassium cyanide is 130 parts then if we divide the potassium cyanide by the tin oxide and multiply it by the 5 grams that we have we would need about 4.33 grams of the cyanide.

$130 \div 150 = 0.867 \times 5 = 4.33$ grams of potassium cyanide.

Every once and a while one might ask, what is the percentage of the composition of a substance? This example uses $2Fe2O_3.3H_2O$ or simplified $Fe_4H_6O_9$. This substance is a hydrate of ferric oxide. So what, in this example would the percentage of iron in this substance be? Again, refer to our diagram below:

Fe_4	=	224	=	56 X 4	
H_6	=	6	=	1 X 6	
O_9	=	144	=	16 X 9	
		374			

Since the molecular weight in total is 374 or 374 parts and we have 224 parts of iron, we can now find the percentage of iron in the substance by the formula:

$$224 \div 374 \times 100 = 59.89\%$$

Every once in a while a solution of copper sulfate known as Blue Stone has to be prepared. This ground down powder is actually crystalized copper sulfate ($CuSO_4.5H_2O$).

So let's say that you had to make up 2 litres of this solution. The formula calls for .001 grams of copper per 1 cc of solution. Therefore how much copper are you going to need? Well you do know that there are 1,000 cc per litre and we need 2 litres or .001 X 2,000 cc = 2 grams. In order to make this amount how much copper (Cu) will be required?

CU	=	63.3		
S	=	32.0		
O	=	64.0	=	16 X 4
$5H_2O$	=	90.0	=	18 X 5
		249.3		

As per the formula above we have 63.3 parts of copper in our solution, therefore we would get $(249.3 \div 63.3 \ \times 2\ grams)$ 7.8769 grams of copper.

This time let's take a look at something a little more complex. Let's say that we have a solution that contains 1 gram of iron for every 100 c.c.'s. If we use the titration method to remove the iron, how much Potassium permanganate are we going to need for the solution? In this process there will be two reactions, the first is dissolving the iron using sulfuric acid. This is shown as:

Fe	+	H_2SO_4	=	$FeSO_4$	+	H_2
↓						
56						

And gives us iron sulfate and hydrogen gas. The second part is to complete the titration which is:

$10FeSO_4 + 2KMnO_4 + 9H_2SO_4 = 2MnSO_4 + 5Fe_2(SO_4)_3 + 2KHSO_4 + SH_2O$						
↓						
K = 39						
Mn = 55						
O_4 = 64						
———						
158 x 2 = 316						

The only substances in this equation above are the two substances under consideration, which are the Potassium permanganate and the iron. So what we have found in the second equation completing the titration is that there are 316 parts of permanganate required for every 10 molecules of iron sulfate. In the first equation we found that there are 56 parts of iron in 1 molecule of iron sulfate. This means that 560 parts of iron is equivalent to 316 parts of the permanganate (10 X 56). Therefore,

$$316 \div 560 \ \times 20 \ grams \ = 11.286 \ grams \ of \ permanganate \ is \ equivelent \ to \ 20 \ grams \ of \ iron.$$

Let’s do another example, but this time this will be in conjunction with an indirect titration. To keep this simple we will use the same criteria as the one before. This time we will use the same equation for dissolving the iron. The second equation is:

$2F2SO_4 + MnO_2 + 2H_2SO_4 = Fe_2(SO_4)_3 + MnSO_4 + 2H_2)$			
↓			
Mn = 55			
O_2 = 32			
87			

In this equation you can now see that the manganese dioxide is equivalent to 112 grams of iron. Therefore ($87 \div 112 \ \times 1 \ = 0.7767 \ grams$) 0.7767 grams is equivalent to 1 gram of iron.

There is one more item that I would like to bring into play here before I close this article. There are times when a one might want to re-evaluate the findings or analysis of a report which was received from an assay lab. As our example here, from an actual assay report on a particular set of samples sent in for analysis. For privacy and other reasons I will not elaborate on the where and when the samples were submitted. We prospector do not disclose such information. However the analysis showed that the sample contained:

Copper Oxide (CuO)-------------------10.58
Iron Oxide (FeO)------------------------15.69
Zinc Oxide (ZnO)------------------------ 0.35
Sulphur Oxide (SO_3)--------------------28.82
Water (H_2O)------------------------------44.71
100.15


As you can see, this does not really tell me much. What I want to do is a comparison. So in order to do this the molecular weights need to be found (using the periodic table) we get:

CuO	63.4 + 16.0	79.3
FeO	56.0 + 16.0	72.0
ZnO	65.3 + 16.0	81.3
SO_3	32.0 + 48.0	80.0
H_2O	2.0 + 16	18.0
		———
		330.6

Next we would need to divide the corresponding percentages with the molecular weights. Here is what we get:

CuO--- $10.58 \div 79.3 = 0.1334$
FeO--- $15.69 \div 72.0 = 0.2179$
ZnO--- $0.35 \div 81.3 = 0.0043$
SO_3---- $28.82 \div 80.0 = 0.3602$
H_2O--- $44.71 \div 18.0 = 2.484$

Now that we have our results as above we need to classify these results. This is accomplished by grouping them into their relative units and combining the values for averaging as shown below (the "R" represents the group as a whole; Cu, Fe, Zn is represented as R and the oxygen as O giving us RO):

Bases		Acids		Water
CuO 0.1334	▬	SO_3 0.3602	▬	H_2O 2.484
FeO 0.2179				
ZnO 0.0043				
———		———		———
RO 0.3556		RO 0.3602		R_2O 2.484

Now that we have the figures, these should be divided by the lowest of the three giving us:

$$0.3556 \div 0.3556 = 1$$
$$0.3602 \div 0.3556 = 1.01 \text{ rounded to } 1$$
$$2.4840 \div 0.3556 = 6.98 \text{ rounded to } 7$$

The formula then becomes $RO.SO_3.7H_2O$. Therefore the sample contained 2/5ths copper, 3/5ths iron, and a tiny bit of zinc.

The previous example was for those that might be or already have a home lab and doing their own unofficial assays for their own determinations. I tried to keep this article geared toward the practice of prospecting and small scale mining whether it is hard rock or place.

If in reviewing this article, you find anything that may be incorrect or missing, please contact me through the contact page and let me know. As a disclaimer, I need to say that I am not a certified Geologist nor am I a Chemist. I too am still learning, and I wish to thank all those (too many to mention here) for all the knowledge and help that you have imparted on me, and for those that have read this article I hope that you enjoyed it and have gained some knowledge from it.