Chapter 5 – Quantities in Chemistry

As you may have begun to see from the way we started, chemistry is a quantitative science involving a great deal of calculations. However, the purpose of these calculations is not merely to get a number, but also to provide quantitative predictions or descriptions of how matter behaves. Correctly calculating the amount of product that is produced in a chemical reaction shows that we understand something about what is really going on in the reaction, and it allows us to use the reaction to produce a desired amount of product. Calculations are tools chemists use in understanding and using the behavior of matter.

One category of chemical calculations involves relationships between quantities of reactants and products based upon relationships given in the balanced equation for any reaction. This is why we will learn how to balance chemical equations in Chapter 6 and kept it as part of our discussions in Chapter 7. Determination of quantities of reactants required for reaction, choosing the amount of reactant necessary to give a desired amount of product, calculation of the concentration of a solution (Chapters 12 and 13), determination of percent composition as a check for purity (Chapter 6), and identification of the empirical and molecular formula of an unknown product (this chapter) all fall into this category, which is generally called **chemical stoichiometry** (Chapters 7, 10, and 12).

Stoichiometry is a more formal term chemists use when they talk about the quantities involved in chemical reactions. It is also a term which is used to describe the *process* of using a chemical equation to calculate the relative masses of reactants and products involved in a reaction. Simply put, stoichiometry is the calculation of quantities in chemical equations/reactions.

First, however, we need some more background.

Section 5-1 – Relative Masses of Elements

1) Sec 5-1.1 – Counting by Weighing
Chemistry is a quantitative science. We will have to analyze the composition of samples of matter and to learn how to be able to measure the amount of matter we have.

I have a friend who owns a driving range. Say he needs to get new range balls each year for the range. How much easier is it to weigh out a quantity of golf balls than to try to count out, say, 8000 balls?

We are returning to (or, better, continuing with) conversion factors, and will be dealing with counts, mass and volume relationships. In chemistry, we call the unifying factor we will use a "MOLE."

2) Sec 5.1-2 – The Mass of an Average Atom

Because atoms are so small, the usual units of mass – the gram and kilogram - are entirely too large to use in normal circumstances. For example, the mass of a single carbon atom is just 1.99×10^{-23} g, but do we want to worry about all the 10^{-23}'s, etc.? To make things easier, chemists have defined a smaller unit for mass, the **atomic mass unit** or **amu**, to use.

Think back to Chapter 2 when we talked about protons, neutrons, electrons, and atoms. At that time we mentioned a "relative" mass for the proton and set that value as equal to 1. The **amu** is related to that concept, so that the "average atomic mass" listed in the Periodic Table for each element is like adding up contributions from all the protons, neutrons and electrons in an atom. In actuality, however, it is based on the carbon-12 isotope (^{12}C) which most chemists <u>define</u> as having a mass of exactly 12.000 amu and, thus, 1 amu is 1/12 of the mass of the carbon-12 isotope and is the mass of a proton.

This means that we can go from the mass of one element to the mass of another element by using conversion factors which involve the atomic masses. For example, if one hydrogen atom has a mass of 1.00 amu and one oxygen has a mass of 16.0 amu, we can get the ratio of: $\frac{1.00\text{ amu}}{16.0\text{ amu}}$

In actuality, we could convert by using the relationship: 1 amu = 1.66×10^{-24} g but most chemists do not do that and we will learn why as this chapter develops.

All the other atomic masses in the Periodic Table are treated the same way and so, in relation to each other, are consistent. This is similar to the idea of multiplying each side of an equation by the same number; this does not change the real value of the equation. The mass of an atom, in amu, is the atomic mass as listed on the Periodic Table. Therefore we can develop something like the following:

H	**O**	**numbers of atoms of each element present**
1.00 amu	16.0 amu	1
2.00 amu	32.0 amu	2
1.00 g	16.0 g	6.02×10^{23}
2.00 g	32.0 g	1.20×10^{24}
1.00 lb	16.0 lb	2.73×10^{26}
2.00 ton	32.0 ton	1.09×10^{30}

Examples:

a. Calculate the mass, in amu, of a sample of sodium that contains 75 atoms. The mass of a sodium atom = 22.99 amu.

b. Calculate the number of aluminum atoms present in a sample that has a mass of 1375.98 amu, if 1 Al atom = 26.98 amu

<u>Section 5-2 – The Mole and the Molar Mass of Elements</u>

3) <u>Sec 5-1.2 – The Definition of the Mole</u>

A mole refers to the amount of substance but it is not something that has a meaning all by itself. (Read: One mole is a lot of things but it is also THE ONE way we can talk about all quantities in chemistry!)

The definition is *the number of atoms (or particles) represented by the atomic mass of an element expressed in grams is a unit known as a* **mole** (The SI symbol is **mol**.) The formal definition goes a step further and concerns an isotope of carbon, ^{12}C. *One mole is defined as the number of atoms in* *exactly* *12 grams of* ^{12}C.

a) Representative Particle or unit refers to whether a substance exists as atoms, ions, or molecules.
   1) The representative particle of most elements is the atom.

   2) There are seven elements whose representative particle is a diatomic molecule. (H_2, N_2, O_2, F_2, Cl_2, Br_2, I_2)

   3) The representative particle of molecular compounds is the molecule.

   4) The representative particle of ionic compounds is the formula unit.

b) Avogadro's Number: One mole of a substance represents 6.02×10^{23} representative particles of that substance.

==> If we have some number of representative particles, we **divide** by 6.02×10^{23} in order to determine the number of moles.

==> If we have some number of moles, we **multiply** by 6.02×10^{23} in order to determine the number of representative particles.

Examples
1) How many moles are there in 1.20×10^{25} atoms of phosphorus?

2) How many molecules are in 0.40 moles of CO_2?

3) How many ammonium ions are in 0.036 moles of ammonium phosphate, $(NH_4)_3PO_4$?

4) Sec 5-2.2 – The Meaning of a Mole

Thus far in our discussion, one mole of a certain element implies two things:

a) The atomic mass expressed in grams. This value is different for each element. This mass is called the **molar mass** of the element. Some refer to this as the **atomic mass** but molar mass will serve as a more general term as we move forward. We find this number on the Periodic Table with the element and each element has a different molar mass.

b) Avogadro's number of atoms or particles (6.022×10^{23}). This value is the same for each element or compound.

5) Sec 5-2.3 – Relationships Among Dozens (the Unit), Number, and Mass

We can easily convert between a unit like the dozen and the number of things present and/or the mass of the whole sample.

Number ----> Dozen ----> Mass

Example: Several years ago I build a deck out of "plastic lumber." In this process I calculated that I would need 1500 screws for the project.

1) If each screw weighs 4.20 g and 1 lb = 453.6 g, how many pounds of screws did I need for the project?

2) When I made my order, screws were available in 5.0 lb boxes, but my supplier determined that it was less expensive to send a 25.0 lb box than the three 5.0 lb boxes I ordered. How many screws did I end up getting?

6) Sec 5-2.4 – Relationships Among Moles (the Unit), Number, and Mass

If we can convert between our usual units, we can do the same things with moles and particles and masses.

Conversion factors	Relationships	Conversion factors
(1) = $\dfrac{1 \text{ mol Na}}{6.022 \times 10^{23} \text{ atoms}}$	1 mol Na = 6.022×10^{23} atoms	(3) = $\dfrac{6.022 \times 10^{23} \text{ atoms}}{1 \text{ mol Na}}$
(2) = $\dfrac{1 \text{ mol Na}}{22.99 \text{ g}}$	1 mol Na = 22.99 g	(4) = $\dfrac{22.99 \text{ g}}{1 \text{ mol Na}}$

Examples:
1) Calculate the mass, in grams, of a sample of sodium that contains 7.5×10^{23} atoms. The mass of one mole of sodium atoms = 22.99 g.

2) Calculate the number of aluminum atoms present in a sample that has a mass of 1375.98 g, if Al has a mass of 26.98 g/mol.

Section 5-3 – The Molar Mass of a Compound

Using moles of atoms instead individual atoms allows us to scale up our measurements into terms that we can use in the real world. Most things around us are made up of compounds, however, and we will learn how chemists scale up these measurements in a similar way.

7) Sec 5-3.1 – The Formula Weight of a Compound

The mass of your computer is the sum of the masses of its individual components. Just the same way the mass of a compound is the sum of the masses of the atoms that make up the compound.

*The **formula weight** of a compound is determined from the number of atoms and the atomic mass (in amu) of each element indicated by a chemical formula.*

Examples – Calculate the formula weight of the following:

1) carbon dioxide, CO_2

2) aluminum oxide, Al_2O_3

8) Sec 5-3.2 – The Formula Weight of Hydrates

Certain ionic compounds have a specific number of water molecules attached to the formula units when they are formed. These compounds are known as ***hydrates*** and have distinctive properties that are different than their ***anhydrous*** (dehydrated or no water) forms. The water of hydration can usually be removed by heating the solid. The formula weight of the hydrate includes the mass of the water molecules.

For example: A common household chemical known as Epsom Salt has the chemical name of **magnesium sulfate heptahydrate** and the chemical formula of $\mathbf{MgSO_4 \bullet 7\ H_2O}$. This dot form does not mean multiply. It is simply how chemists show in a formula the presence of the seven water molecules because they are still distinct water molecules and have not been changed. The formula mass of $MgSO_4 \bullet 7\ H_2O$ is calculated by summing the atomic masses of magnesium, sulfur, four oxygens, and seven waters.

1 magnesium	24.31 amu
1 sulfur	32.07 amu
4 oxygen	64.00 amu
7 water	126.11 amu
	246.49 amu

9) Sec 5-3.3 – The Molar Mass of a Compound

The formula weight represents the mass of one molecule or formula unit. We again need to scale this up so that we can have workable measurements that we can use in the laboratory. We do this by extending the definition of a mole to include compounds. *The mass of one mole (6.022 x 10^{23} molecules or formula units) is referred to as the* ***molar mass of the compound*** *and is the mass of the molecule or formula unit expressed in grams*. As we noted with atoms of elements, the molar masses of various compounds differ, but the number of molecules or formula units remain the same.

Very simply, the "molar mass" is the mas of one mole of whatever substance (element, molecular compound, or ionic compound) we are interested in.

Examples – Calculate the molar mass of the following:

1) glucose, $C_6H_{12}O_6$

2) aluminum sulfate, $Al_2(SO_4)_3$

10) The Volume of 1 Mole of a Gas [Not here in your book.]
The volume of 1 mole of any gas measured at 0°C (**standard temperature**) and 1 atmosphere pressure (**standard pressure**) is 22.4 liters. (The term Molar Volume is often used for the volume of 1 mole of a gas at STP.)

[1 mole of a gas = 22.4 L at STP]

==> If we have some volume of a gas at STP, we **divide** by 22.4 liters in order to determine the number of moles.

==> If we have some number of moles of a gas at STP, we **multiply** by 22.4 liters in order to determine the volume of the gas at STP.

Examples

a) What is the volume at STP of 0.48 moles of methane, CH_4?

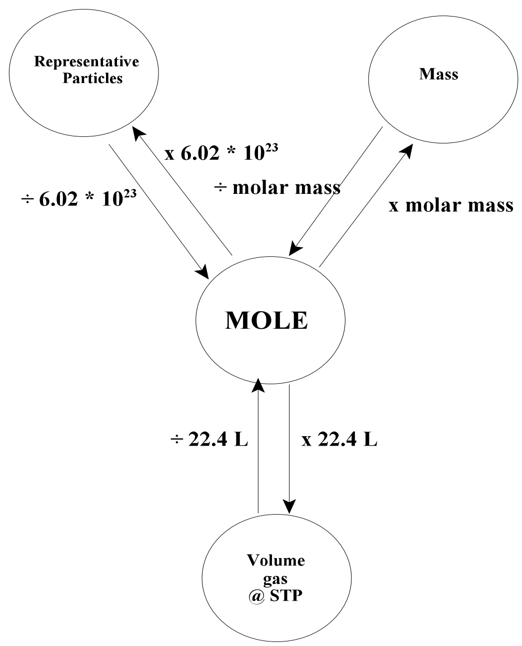
b) How many moles are in 89.6 L of Neon, Ne?

c) What is the mass of 0.448 L of oxygen gas, O_2 (volume measured at STP)?

d) What is the density of CO_2 gas at STP in g/L?

e) If the density of a gas is 0.714 g/L at STP, what is its molecular mass?

11) Mr Weinkauff's Summary of Mole Calculations [Not in your book!]
There are all kinds of ways to simplify thinking about calculating to and from moles using any quantity you might have or be looking for. This is the simplest I have seen. At times it has helped me remember some basic concepts.



One of the beauties of this particular visual model is the idea that whenever you are at MOLES you multiply to get to the other value. That is, when you go **OUT** from the center you multiply.

Likewise, if you have grams, particles, or volume at STP you always divide to get to MOLES. That is, when you are on the outside you divide to get to the center. (We have not covered this but mentioning it now helps to complete the drawing. We will get to gases and this later in Chapter 10, and explain what it means then.)

Also you should note that by following this diagram you are reminded that you **CANNOT** go directly from particles to mass (or visa versa or with gases) in calculations. You **MUST** go through moles.

12) Summary of Calculations to calculate the number of moles (n) of what is given

1) Mass (convert to grams if necessary): $n = \frac{\text{mass (g)}}{\text{molar mass}}$

2) Volume of a Liquid (use density to get mass in grams):
density = $\frac{\text{mass (g)}}{\text{volume (mL)}}$ or mass (g) = density x volume(mL)
And then, as above: $n = \frac{\text{mass (g)}}{\text{molar mass}}$

3) Molecules: $n = \frac{\text{\# of molecules}}{6.02 \times 10^{23}}$

4) Volume of a Gas at STP (convert volume to liters if necessary): $n = \frac{\text{volume (L)}}{22.4\text{ L}}$

Examples:

1) How many grams are there in 5.80 moles of calcium carbonate, $CaCO_3$?

2) How many moles are there in 8.80 g of carbon dioxide, CO_2?

3) How many liters will 8.80 g of carbon dioxide, CO_2, occupy at STP?

4) How many molecules are there in 500 g of sulfur dioxide, SO_2?

5) What is the mass in grams of 100 molecules of chlorine, Cl_2?

Section 5-4 – The Composition of Compounds

As we look at formulas, it may occur to us that everything is not equal. That is, one oxygen atom and two hydrogen atoms gives us one water molecule. How can we use this?

13) Sec 5-4.1 – The Mole Composition of a Compound

When we look at a compound, we can separate a quantity of the compound expressed in moles into the number of moles of each element of the compound that is present. To do this we establish a **mole ratio** which shows the *relationship between the number of moles of a particular element and a mole of the compound containing that element.*

The Composition of One Mole of H_2SO_4

Number of Atoms		Moles of Atoms		Mass of Atoms
1.204×10^{24} H atoms	←	2 mol H	→	2.016 g H
6.022×10^{23} S atoms	←	1 mol S	→	32.07 g S
2.409×10^{24} O atoms	←	4 mol O	→	64.00 g O
4.215×10^{24} atoms in		7 mol atoms in		
6.022×10^{23} molecules	←	1 mole of molecules	→	98.09 g

14) Sec 5-4.2 – The Mass Composition of a Compound

We can use the mole ratio to help us determine the masses of the elements present in a particular sample of a compound.

Example: How many grams of iron are there in 250 g of Fe_2O_3?

15) Sec 5-4.3 – The Percent Composition of a Compound

A common way of expressing the composition of elements in a compound is percent composition. **Percent composition** *expresses the mass of each element per 100 mass units of compound.*

$$\%\text{ mass of element E} = \frac{\text{grams of element E}}{\text{grams of compound}} \times 100$$

Example: Compounds containing chlorates are known to decompose by giving off oxygen when heated. A student heated 0.800 g of a chlorate and obtained a residue that had a mass of 0.600 g. What is the percent of oxygen in the chlorate?

Occasionally you may want to calculate the percentage composition of a known compound. The percentage of an element in a compound can be calculated from atomic masses if the formula of the compound is given, using the following relationship.

$$\%\text{ mass of element A} = \frac{\#\text{ of atoms of element A} \times \text{molar mass of A}}{\text{molar mass of compound}} \times 100$$

Example: What is the percentage of phosphorus in calcium phosphate, $Ca_3(PO_4)_2$?

Section 5-5 – Empirical and Molecular Formulas

16) Sec 5-5.1 – Empirical Formulas

With some molecular compounds when you calculate the percentage of each element, the result does not give an idea of the distinct compound you are interested in. Remember that the **molecular formula** *of a compound is the actual number of atoms present in the compound.* For example, acetylene (C_2H_2) and benzene (C_6H_6) are two different molecular compounds (the first is a gas and the second is a liquid) but both have 92.26% carbon and 7.74% hydrogen. This is because they have the same empirical formula. *The* **empirical formula** *gives the simplest whole number ratio of the elements in a compound (lowest or smallest whole number ratio of moles of atoms in a compound).* The empirical formula for both of these compounds is CH. [Note that the empirical formula does not have to exist as something by itself.]

If you have a formula you can determine the empirical formula by dividing each subscript by a common factor. So, for C_2H_2 you divide by 2 to get the empirical formula of CH, and with C_6H_6 you divide by 6.

Likewise, formaldehyde (CH_2O) and paraformaldehyde ($C_3H_6O_3$) both have an empirical formula of CH_2O but they are different compounds. It turns out that the molecular formula for formaldehyde is also its empirical formula. And you divide $C_3H_6O_3$ by 3 to get the same empirical formula.

You should realize that for almost all ionic compounds the empirical formula is the formula we use because of the way we write the formula unit (that is, the smallest whole number ratio of the atoms present).

17) Sec 5-4.2 – Calculating Empirical Formulas

Remember that a formula tells us the number of atoms of each element present in a compound and, as we saw earlier, the number of moles of each element in a mole of a compound. Calculating the empirical formula from experimental data requires us to calculate the number of moles of each element present in the sample and then compare these.

Steps to Calculating an Empirical Formula

1) If the percentage composition of the compound is given, use the percentages to find the mass of each element that would be present in a 100 g sample of the compound. Thus the percentage becomes the mass expressed in grams. (In some cases you may be given the mass of each element.)

2) Determine the number of moles of each element present in the compound by dividing the mass of each element by its atomic mass.

3) To determine the simplest whole number ratio, divide the number of moles of each element by the smallest number of moles that is present. If this does not give a whole-number ratio (within 0.1 of a whole number), multiply by a number like 2 or 3 to make the numbers whole numbers.

Examples

1) Calculate the empirical formula of a compound that contains 2.0 g of calcium and 8.0 g of bromine.

2) Calculate the empirical formula of a compound given the following percentage composition: 15.8% Al, 28.1% S, and 56.1% O.

3) Calculate the empirical formula of a compound that contains 39.99% C, 6.71% H and 53.28% O.

18) Sec 5-4.3 – Determining the Molecular Formula of a Compound

As noted above for CH_2O and $C_3H_6O_3$, the molecular formula may or may not be the same as the molecular formula. The molecular formula is the actual formula of the compound. To determine the molecular formula we must determine the number of "empirical units" that are present in the molecule because it is either the same as or some whole number multiple of the empirical formula.

In order to determine this we need to know both the molar mass of the compound (g/mol) and the mass of the empirical formula (g/emp unit). The ratio of these two values must be a whole number and is the multiplier that we apply to the empirical formula.

Examples:

1) What is the molecular formula of a compound that is 92.3% carbon and 7.7% hydrogen. The compound's molar mass is 78 g/mol.

2) What is the molecular formula of a compound that has 37.83% C, 6.35% H and 55.83% Cl. It has a molar mass of about 127.0 g/mol.

For our current work I will have to tell you the molar mass of the compound for you to be able to complete the problem. However, in a later chapter we will learn a method to determine the molar mass in some circumstances from other data.

Remember: **MOLAR MASS** is a general term that covers the more specific terms of atomic mass, formula mass, and molecular mass.