Chapter 7 – Quantitative Composition of Compounds

One question of great importance to chemists is how much of a substance is present in a sample. It turns out that the answer is a little more complicated than what first comes to mind. If the sample is water, chances are the amount is measured as volume. If the sample is a box of cornflakes, the amount is likely measured as weight. Thus, one method of indicating how much of a substance is present is by measuring the amount present using an appropriate measuring device. If one takes a step back and thinks about it for a little while, a second way of expressing amount comes to mind, which is counting. Looking at our last two examples, there is no way at all to count the amount of water present in a sample. One could count the number of cornflakes in a box, but it would take a very long time and there would be the question of how do you deal with broken flakes. Thus, the only practical method of answering how much of these materials are present is by using a weight or volume measurement.

If the question is eggs, however, then we always use counting. (Have you ever heard of a recipe calling for a weight or volume of eggs?) Likewise, we always discuss the amount of paper present using counting. In both cases, there is no reason why we couldn't use weight as the method, but it is never done. Why not?

The answer is convenience and accuracy. Convenience because if one is making an omelet, it is much easier to get ready if one is told it needs 3 large eggs, rather than 171 g of eggs. Likewise, a ream of paper has 500 sheets, but there is some variation in the weight of each sheet. If paper was sold by weight instead of number of sheets, some packs would have 499 sheets, most 500, and some 501 sheets. If doing large copy jobs and loading full packages of paper into a photocopier, having the exact number of sheets is very important.

In chemistry, we usually use measured values to express how much of a substance is present. However, there are times when counting is much easier. For example, consider the reaction:

$$2H_{2\,(g)} + O_{2\,(g)} \rightarrow 2\,H_2O_{(\ell)}$$

One could remember than 4 grams of hydrogen react with 32 grams of oxygen to produce 36 grams of water, but it's much easier to remember that 2 molecules of hydrogen react with a molecule of oxygen to yield two molecules of water.

In this chapter we explore the counting aspect of chemistry in some detail and examine how to move between counting and measuring.

7.1 The Mole

As you know, individual atoms have incredibly small masses, which means that any amount of a material that you can see has an unimaginably large number of atoms present. In Chapter 5, the atomic mass unit was introduced to avoid working with very small masses, a measured quantity. The mole addresses counting the extremely large number of particles present in any macroscopic sample.

We routinely use collective counting terms such as dozen or a ream (500). Collective terms allow us to work with increasingly large quantities more easily. In a sense, weighing systems do this. For example, which is easier to think about: a person weighs 150 lbs or 2,400 ounces? A small car weighs about 1 ton = 2,000 lbs = 32,000 ounces. When counting atoms, the collective term dwarfs any of these terms. Recall that carbon-12 was used to establish the relationship between the mass of atoms in grams vs. their masses in amu's. For counting particles, the number of atoms of carbon-12 in 12.0 g of carbon-12 defines the collective term, called the ***mole****. A mole of a substance contains 6.022 x* 10^{23} *atoms.*

Literally, this number is so large that you cannot really comprehend it. What is important to remember when using it is that it works functionally like a dozen, just far larger. So, when thinking about the mole, if you substitute "dozen" for "mole" in the sentence and it makes sense, you are probably using mole correctly.

On the periodic table, each block has at least three pieces of information. The atomic symbol, number, and mass. The mass never has units because it is added when used. If only one atom is present, then the unit is amu, if a mole of atoms, then the unit is grams. The following two problems should help show how the mole is useful in calculations.

How many molecules of oxygen are present in 10.0 g?

$$molecules_{O2} = (10.0\ g_{O2})\left(\frac{6.022\ x\ 10^{23} molecules_{O2}}{32.00\ g_{O2}}\right) = 1.89\ x\ 10^{23}\ molecules_{O2}$$

How many moles of oxygen molecules are present in 10.0 g?

$$moles_{O2} = (10.0\ g_{O2})\left(\frac{1\ mole_{O2}}{32.00\ g_{O2}}\right) = 0.0312\ mole_{O2}\ \ (3.12 \times 10^{-2}\ mole_{O2})$$

7.2 Molar Mass of Compounds

As important as is atomic mass, the vast majority of pure substances are compounds. Unlike for elements, where the atomic masses are printed on the periodic table, the mass of a mole of a pure substance (its molar mass) must be calculated. Fortunately, the calculation is straightforward. Begin with the formula and then use the number and mass of each kind of atom to determine the mass of the whole. For example, what is the molar mass of silicon tetrachloride?

$$molar\ mass_{SiCl4} = (1\ mol_{Si})\left(\frac{28.086\ g_{Si}}{1\ mol_{Si}}\right) + (4\ mol_{Cl})\left(\frac{35.453\ g_{Cl}}{1\ mol_{Cl}}\right) = 169.898\ g$$

Always do these calculations to the correct number of significant digits. If they aren't all needed, the molar mass can be truncated to the right number of digits. (Nearly all books, including this one, routinely report molar masses (frequently molecular weights, MW) to only the one-hundredths place. Do not do this as sometimes the extra digits matter.)

Elemental molecules represent an area of significant confusion for many students. For example, the molar mass of iron is always 55.847 g/mol. In contrast, the molar mass of nitrogen isn't clear because the atom weighs 14.0067 g/mol, but the molecule, N_2, which is how nitrogen is found in nature weighs 28.0134 g/mol. Sometimes problems explicitly request the value for one or the other, but most times it must be inferred. If the element is used in a reaction or occurs in its natural form, use the mass of the molecule.

Just as for the elements, moving between masses and moles is a very common calculation in chemistry. For example, how many moles of silicon tetrachloride, SiCl4, in a 250 g sample?

$$moles_{SiCl4} = (250\ g_{SiCl4})\left(\frac{1\ mol_{SiCl4}}{169.898\ g_{SiCl4}}\right) = 1.47\ mol_{SiCl4}$$

7.3 Percent Composition of Compounds

Consider the molecule water, H_2O. It contains how much hydrogen and oxygen? There are two ways to answer this question. As the question is written, the first answer that comes to mind is probably: there are two hydrogen and one oxygen atom in water. A second answer would be there are 2.01494 amu of hydrogen and 15.9994 amu of oxygen in it. Both answers are correct because they approach the question from different perspectives and both are useful in different settings.

A third way to answer the question employs percentages. The water molecule is also 11.19% hydrogen by mass and 88.81% oxygen by mass. In the lab, determining the exact mass of each element turns out to be difficult many times, while determining the percentage of each element present is relatively simple. We begin with the calculation that yields the values for hydrogen and oxygen in water.

$$\text{molar mass}_{H2O} = (2\ \text{mol}_H)\left(\frac{1.00794\ g_H}{1\ \text{mol}_H}\right) + (1\ \text{mol}_O)\left(\frac{15.9994\ g_O}{1\ \text{mol}_O}\right) = 18.0153\ g$$

$$\%H = \frac{(2\ \text{mol}_H)\left(\frac{1.00794\ g_H}{1\ \text{mol}_H}\right)}{18.0153\ g} \times 100\% = 11.19\%_H$$

$$\%O = \frac{(1\ \text{mol}_O)\left(\frac{15.9994\ g_O}{1\ \text{mol}_O}\right)}{18.0153\ g} \times 100\% = 88.81\%_O$$

alternatively $\%O = 100\% - 11.19\%H = 88.81\%_O$

There are a three points that warrant comment:

1) The percentages are truncated to the hundredth's place. This is standard practice because the experiment that measures percent composition is only that accurate.
2) There are two ways to calculate the final percentage, either the same way as the other elements or as what is left of the original 100%. The former method is better because if you make a calculational error, it is more likely to appear in the more involved calculation.
3) The percentages for all elements should total close to 100%, but because of rounding error may not exactly equal 100%. In general, the total should be between 99.98% and 100.02%. Larger differences suggest a calculational error.

7.4 Calculating Empirical Formulas

Percent composition has significant practical value in chemistry. When one attempts to make a new compound, the first question that arises is "What have I made?" The chemist knows what s/he was trying to make, but it could easily be something different. The most basic process to determine the identity of a material is elemental analysis. There are various experiments done as *part of the process, but basically the goal is to determine the percent composition of the sample. With that information, the empirical formula of the sample compound can be determined. The empirical formula of a compound gives the smallest whole-number ratio of each type of atom present in a compound. Compounds also have molecular formulas, which have the actual number of each type of atom present.*

The calculation of an empirical formula follows the following steps:

1) *Confirm the percentages total to 100%.*
2) *Assume there are 100 g of compound present. (Then the amount of each element present in grams will equal the percentage of that element present.)*
3) *Calculate the number of moles present of each element. (Make sure to use the element in elemental form (e.g. oxygen as 15.9994 g/mol **not** 31.9998 g/mol).*
4) *Calculate the molar ratios, dividing by the element with the smallest number of moles present. (Retain units throughout the process.)*

Example: *An unknown compound is found to be composed of 40.0% carbon, 6.7% hydrogen, and 53.3% oxygen. What its empirical formula?*

$$mol_C = (40.0\ g_C)\left(\frac{1\ mol_C}{12.011\ g_C}\right) = 3.33\ mol_C$$

$$mol_H = (6.7\ g_H)\left(\frac{1\ mol_H}{1.0079\ g_H}\right) = 6.65\ mol_H$$

$$mol_O = (53.3\ g_O)\left(\frac{1\ mol_O}{15.9994\ g_O}\right) = 3.33\ mol_O$$

molar ratios:

$$C: \frac{3.33\ mol_C}{3.33\ mol_C} = 1.00$$

$$H: \frac{6.65\ mol_H}{3.33\ mol_C} = 2.00\ mol_H \text{ per } mol_C$$

$$O: \frac{3.33\ mol_O}{3.33\ mol_C} = 1.00\ mol_O \text{ per } mol_C$$

The empirical formula is CH_2O.

The problem with empirical formulas is that they provide only the relative number of atoms in the molecule, not the actual. For example, there are several compounds that have the empirical *formula CH_2O, two of which are formaldehyde (CH_2O) and glucose ($C_6H_{12}O_6$). You don't have to be a chemist to appreciate that you don't want to mix these compounds up. In Section 7.5, we will discuss how to determine the molecular formula of a compound.*

Note that with one exception, all of the numbers in this example have units. Be careful in rounding the molar ratios. You should round numbers very close to integers (e.g. 0.97 rounds to 1), but numbers close to 0.25, 0.33, and 0.5 should be treated differently. In these cases, all ratios are multiplied by a factor to yield whole number values. e.g. A compound has the following ratios: Fe = 1.00, O = 1.33 oxygen atoms per iron atom. Multiply through by 3 to get Fe_3O_4. Aluminum oxide (Al_2O_3) has a ratio of 1.50 mol_O per mol_{Al}.

One common variant on this problem provides the actual masses of the elements, rather than the percentages. In this case, just plug those masses in just as the percentages are in the previous example.

7.5 Calculating the Molecular Formula from the Empirical Formula

How chemists obtain the percentages is not part of the course, but knowing the method might be interesting or helpful in understanding the process fully. Each element has a different experiment that yields its percentage. Consider a compound that contains only hydrogen and carbon, such as butane lighter fluid. A weighed sample is burned, which produces carbon dioxide (CO_2) and liquid water (H_2O). The water can be weighed directly and the carbon dioxide can be captured and weighed. Since the only source of hydrogen in the water is the compound, the mass of the hydrogen in the water equals the mass in the butane. The same is true of the carbon in the CO_2. With the masses of H and C known, the percentage of each in the compound is calculated.

As mentioned above, the empirical formula only gives the relative number of atoms of each element, not the actual number. For example, when performed on formaldehyde (CH_2O) and glucose ($C_6H_{12}O_6$), the combustion experiment yields the same percentages for all three elements. A second experiment must be conducted to determine the actual (molecular) formula of the compound. Again, there are different experiments that determine the actual mass of the compound. (For example, the smaller, lighter formaldehyde evaporates more rapidly than glucose and that difference can be used *to determine the molecular mass.)*

Example: *For the compound in the previous example, if the molecular weight is about 180 g/mol, what is its molecular formula?*

The empirical weight of CH_2O is 30 g/mol.

$$\frac{MW}{EW} = \frac{180\ g/mol}{30\ g/mol} = 6.0$$

Thus, there are 6 empirical units in each molecule $\Rightarrow C_6H_{12}O_6$

August 21, 2023