Chapter 3 – Composition of Substances and Solutions

This chapter addresses two basic concepts: 1) the masses of molecules and salts at both the atomic and macroscopic levels and 2) the number relationship between reacting species. Read Section 3.1 on your own. We'll return to all of its content later in the notes.

3.1   Formula Mass and the Mole Concept

As you've already surmised, on the macroscopic scale the amu is as inconvenient as the gram is at the atomic scale, so we use the gram for "normal" scale situations. However, it would be convenient to be able to move easily between these scales. The conversion factor 6.022×10^{23} allows for such easy movement.

As your book observes, even small amounts of material contain unimaginably large numbers of atoms. For example, one teaspoon of water holds 10^{23} molecules. If you can see it, a sample of anything contains at least a million, million, million molecules. For that reason, a collective term was developed. The <u>mole</u> contains 6.022×10^{23} items (<u>Avogadro's number</u>). Memorize this value. The mole is similar to the dozen (12 items) and gross (144 items) in that it is a counting term. Technically, a mole contains the number of atoms in exactly 12 g of ^{12}C. Remember that "exactly" means there is no error in this number. Using the g/amu conversion factor means if one carbon-12 atom weighs exactly 12 amu, then one mole of ^{12}C weighs exactly 12 g. Therefore, one chooses the mass units based on the scale one works on. This is why the periodic table does not have units next to the masses.

Your book begins with formula masses in this section (p. 132), then later discusses molar masses (p. 135). In real life though, "formula mass" is rarely used and the molar mass does double duty; in

fact we usually say molecular weight (MW) even though this term is technically incorrect. <u>All can be thought of as the sum of the masses of the atoms that compose one unit of a material</u>. Thus, for glucose, $C_6H_{12}O_6$:

$$MW_{glucose} = (6\ atoms_C)(\frac{12.011\ amu}{atom_C}) + (12\ atoms_H)(\frac{1.0079\ amu}{atom_H}) + (6\ atoms_O)(\frac{15.9994\ amu}{atom_O})$$

$$=180.157\ amu$$

Note that I don't round off to the tenths place like the book does in all of its examples. You shouldn't either for two reasons: 1) with calculators it isn't worth the trouble and 2) in some cases, you may make a significant figure error.

Example*: How many moles of glucose, $C_6H_{12}O_6$, are in 1.00 g? How many molecules? How many carbon atoms?*

$$MW_{C6H12O6} = 180.157\ amu/molecule \rightarrow MW_{C6H12O6} = 180.157\ g/mole$$

$$mol_{C6H12O6} = (1.00\ g)\left(\frac{1\ mol}{180.157\ g}\right) = 5.55\ x\ 10^{-3}\ mol$$

$$molecules_{C6H12O6} = (1.00\ g\ g)\left(\frac{1\ mol}{180.157\ g}\right)\left(\frac{6.022\ x\ 10^{23}\ molecules}{mol}\right)$$

$$= 3.34\ x\ 10^{21}\ molecules$$

$$atoms_C = (1.00\ g)\left(\frac{1\ mol}{180.157\ g}\right)\left(\frac{6.022\ x\ 10^{23}\ molecules}{mol}\right)\left(\frac{6\ atoms_C}{molecule}\right)$$

$$= 2.00\ x\ 10^{22}\ atoms_C$$

When discussing materials, be careful to think about what is really being asked for in the text. In particular, if nitrogen is listed as a product of reaction, what is typically meant is molecular nitrogen, or N_2, not atomic nitrogen (N). There is similar ambiguity in other materials (e.g. oxygen and chlorine) and you should learn to anticipate what is expected in these situations.

3.2   _Determining Empirical and Molecular Formulas_

Percent composition is a common and very useful calculation in chemistry. It provides the elemental composition as the percent of total molecular weight. When a new compound is prepared, its elemental composition is usually determined. The following calculation provides the expected composition based on molecular formula. For glucose:

$$\%C = \frac{(6\ atoms_C)\left(\frac{12.011\ amu}{atom_C}\right)}{180.157\ amu} \times 100\% = \qquad 40.00\%$$

$$\%H = \frac{(12\ atoms_H)\left(\frac{1.0079\ amu}{atom_H}\right)}{180.157\ amu} \times 100\% = \qquad 6.71\%$$

$$\%O = \frac{(6\ atom_O)\left(\frac{15.9994\ amu}{atom_O}\right)}{180.157\ amu} \times 100\% = \qquad \underline{53.28\%}$$
$$99.99\%$$

There are three points worth noting here: (1) Substituting grams for amu gives exactly the same numerical answers. Use whichever unit the problem requires. (2) You should add the percentages together and make sure they total 100% ± 0.02%. There will frequently be a very small deviation from 100% because of rounding, but it should never be much larger than a couple hundredths of a percent. (3) By convention, percent composition is almost always reported to a maximum accuracy of hundredths of a percent, even though the calculation may be more accurate. This is because percent composition calculations are usually used in the determination of the identity of unknown materials. It is quite difficult to obtain materials more than 99.9% pure and, combined with experimental error in making the measurements, hundredths of a percent does quite well for almost all purposes.

Unlike many calculations you do, this is one which is done in the reverse direction as often as the forward direction. That is, we often start with the percentages and try to determine the number

of atoms of each element present. For example, we can burn a sample containing C & H and collect and weigh the CO_2 & H_2O produced. From their weights, the amount of C and H in the original sample can be determined. Similar experiments are performed for other elements. Using elemental analysis percentages allows one to calculate the _empirical formula_ of a compound.

The empirical formula presents the relative number of each kind of atom in the compound. In contrast, the _molecular formula_ presents the actual number of atoms in the compound. For example, glucose has a molecular formula of $C_6H_{12}O_6$, while it has an empirical formula of CH_2O. This distinction is important. If you burn formaldehyde (CH_2O) and glucose, they yield the same percentages of C, H, and O, so they yield the same empirical formula, yet are clearly very different materials.

The calculation 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. Its molecular weight was measured as 180 g/mol. What are its empirical and molecular formulas?

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

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

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

molar ratios:

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

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

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

The empirical formula is CH_2O.

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.

If you also have the molecular weight of the material, you can determine the molecular formula. When going from empirical formula to molecular formula, all of the <u>subscripts</u> are multiplied by a whole number. *This is the <u>only</u> time it is permissible to change the subscripts on a formula.*

Example: In the previous problem you were told the molecular weight was about 180 g/mol, you

calculate the molecular formula as follows:

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 $\Rightarrow C_6H_{12}O_6$

3.3   *Molarity*

Recall from Chapter 1 that a <u>solution</u> is a homogeneous mixture at both the macroscopic and microscopic levels. A <u>solvent</u> is the liquid present in largest quantity in a liquid solution. All other materials are dissolved in the solvent and are called <u>solutes</u>. In <u>aqueous</u> solution, the solvent is water. Aqueous means "dissolved in water."

The composition of a solution is most frequently described in terms of concentration. <u>Concentration</u> is the amount of one material dissolved in a second material. The most common and important unit for describing the concentration of a solution is molarity. The unit of molarity is moles of solute per liter of solution and is abbreviated "M." Placing the dissolved species in square brackets also means molar concentration (see below). Note that the volume of solution is used, not

$$\text{concentration} = \frac{\text{moles of solute}}{\text{volume of solution (in liters)}}$$

just the solvent added. If large amounts of solute are added to pure solvent the total volume will increase, but if small amounts are added either an increase or decrease may occur. (A small solute species might draw solvent molecules towards itself, thus causing a small shrinkage.) These units allow convenient comparison of reactants in different solutions through balanced equations. We'll go over other concentration units as we need them.

Example: What is the molarity of a solution that contains 17.4 g NaCl per 112 mL solution?

$$[NaCl] = (17.4\ g)\left(\frac{1\ mol}{58.44\ g}\right)\left(\frac{1}{112\ mL}\right)\left(\frac{1000\ mL}{L}\right) = 2.66\frac{mol}{L} = 2.66\ M$$

Likewise, the mass of a solute or volume or solvent can be obtained if 2 of the 3 (M, mass, vol) are

known.

It is important to keep in mind that the terms "dilute" and "concentrated" are relative and there is no strict definition of either. A term that is useful when discussing solubility is "saturated." A solution is <u>saturated</u> when no more of the solute will dissolve at a particular temperature. This will be discussed at length in CHM 212, but it's a term you will hear in CHM 217. A solution is "unsaturated" if less than the maximum amount has dissolved. Another important thing to remember is that saturated solutions are not necessarily concentrated and unsaturated solutions are not necessarily dilute. For example, you can grind up some chalk and add it to water and saturate the solution. It will be dilute. Make a gallon of a saturated sodium chloride solution. It is concentrated. Add a teaspoon of water and it's no longer saturated, but it's still concentrated.

When an ionic solid dissolves, it exists in solution entirely as ions. For convenience we write 0.1 M NaCl, but in reality no NaCl actually exists in solution. The solution consists of 0.1 M Na^+ and 0.1 M Cl^-. For 0.1 M Na_2CO_3:

Example: $[Na^+] = 0.2\ M$ and $[CO_3^{2-}] = 0.1\ M$

<u>Dilution</u> is the process of making a solution less concentrated, usually by adding solvent to a solution. In this situation, the total amount of solute remains the same. A convenient equality can be used to calculate the concentration after a solution has been diluted.

$M_c V_c = M_d V_d$

This allows you to calculate the concentration of a solution after more solvent has been added, or more usefully, to calculate how much solvent must be added to an existing solution to dilute to a new concentration.

Example: What is the concentration of a solution after 25.0 mL of the previous sodium chloride

is added to 125 mL of water? (Assume the volumes are additive.)

$(2.66 \text{ M})(25.0 \text{ mL}) = M_f (1.50 \times 10^2 \text{ mL})$

$M_f = 0.443 \text{ M}$

How much water must be added to 50.0 mL of the original NaCl solution to make it 1.00 M?

$(2.66 \text{ M})(50.0 \text{ mL}) = (1.00 \text{ M})V_f$

$V_d = 133 \text{ mL}$

Volume added = 133 mL - 50 mL = 83 mL

One thing you might have noticed is that the volume term in molarity is L and the volumes used in the examples are mL. We can get away with this because of the equality. In each case, either the concentration or volume units will cancel.

3.4   Other Units for Solution Concentrations

There are numerous other concentration units used in chemistry, but these other units are employed in specific situations and not use used in as widespread of a way as molarity. There are five such units introduced here, four of which have names that are largely self-explanatory.

Mass percentage is the ratio of the mass of a solution component relative to the mass of the entire solution.

$$\text{mass percent}_{component} = \frac{component\ mass}{solution\ mass} \times 100\%$$

This is sometimes called weight percent and can be abbreviated (w/w)%. This unit is usually employed for moderately concentrated solutions.

Volume percentage is the ratio of the volume of a solution component relative to the volume of the entire solution. This unit is only employed with solutions where at least one solute is a liquid.

$$\text{volume percent}_{component} = \frac{\text{component volume}}{\text{solution volume}} \times 100\%$$

This is frequently abbreviated (v/v)%. This unit is usually employed for moderately concentrated solutions.

Parts per million and parts per billion are similar to mass percentage, but for very dilute solutions and only refer to the solute(s). Thus, the equations are:

$$\text{parts per million}_{component} = \frac{\text{component mass}}{\text{solution mass}} \times 10^6$$

$$\text{parts per billion}_{component} = \frac{\text{component mass}}{\text{solution mass}} \times 10^9$$

Although solutions can be intentionally prepared this dilute, these units are more typically associated with the amount of an impurity/contaminent is present in a sample.

Skip the mass/volume unit.

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