Topic 6: Common Lab Calculations

Written by
Danielle M. Solano
Department of Chemistry & Biochemistry
California State University, Bakersfield

As part of your labs, you will often have to calculate the amounts of the different reagents you will be using and convert from one unit of measure to another. Additionally, you will have to calculate the theoretical yield of your reactions, and the percent yield of your reactions once you have isolated the product.

Calculating Grams from Molecular Weight

If you are given the amount of material you need in moles, you will need to convert this value to grams so you know how much material to weight out. For example, let's say you need 5.0 mmoles of benzoic acid. First, you will need to lookup the molecular weight of benzoic acid (it is 122.12 g/mol). Here's how you would calculate the amount of grams you need:

$$\frac{122.12\ \text{g}}{\text{mol}} = \frac{122.12\ \text{mg}}{\text{mmol}}$$

$$\frac{122.12\ \text{mg}}{\text{mmol}} \times 5.0\ \text{mmol} = 610\ \text{mg} = 0.61\ \text{g}$$

Calculating Moles from Concentration

If you are given the amount of material you need in volume, you will need to convert this value to moles to do other calculations (such as calculating molar equivalents or determining the limiting reagent). For example, let's say you need 6.0 mL of HCl. First, you need to know the concentration of the HCl solution. In this example, let's say we have 2.0 M HCl. Here's how you would calculate the moles in 6.0 mL of solution:

$$2.0\ \text{M} = \frac{2.0\ \text{mol}}{\text{L}} = \frac{2.0\ \text{mmol}}{\text{mL}}$$

$$\frac{2.0\ \text{mmol}}{\text{mL}} \times 6.0\ \text{mL} = 12\ \text{mmol} = 0.012\ \text{mol}$$

Adjusting the Concentration of a Solution

If you need a certain concentration of a solution, and you are given a more concentrated solution, you will need to dilute the solution to the correct concentration. For example, let's say you need 6.0 mL of 2.0 M HCl, but you only have 3.0 M HCl. You will need to use the equation $M_1V_1 = M_2V_2$ to calculate the volume of 3.0 M HCl needed. In this example, our initial concentration (M_1) is 3.0 M, our final concentration (M_2) is 2.0 M, and our final volume (V_2) is 6.0 mL.

$$3.0\ \text{M} \times V_2 = 2.0\ \text{M} \times 6.0\ \text{mL}$$

$$V_2 = \frac{2.0\ \text{M} \times 6.0\ \text{mL}}{3.0\ \text{M}} = 4.0\ \text{mL}$$

So you need to add 4.0 mL of 3.0 M HCl to a graduated cylinder, and then add deionized water to reach the 6.0 mL mark to prepare the necessary amount of your 2.0 M solution.

Converting Grams to Moles

If you are given the amount of material you need in grams, you will need to convert this value to moles so you can determine the limiting reagent in your reaction. For example, let's say you start with 3.05 g of sodium benzoate. First, you will need to lookup the molecular weight of sodium benzoate (it is 144.11 g/mol). Here's how you would calculate how many moles this is:

$$3.05\ \text{g} \times \frac{\text{mol}}{144.11\ \text{g}} = 0.0212\ \text{mol} = 21.2\ \text{mmol}$$

Determining the Limiting Reagent

If all of your reagents are reacting in a one-to-one ratio, this is simply going to be the reagent with the smallest number of moles being used. For example, let's consider the reaction of sodium benzoate and HCl (as shown in Lab 5). In this reaction, every mole of sodium benzoate that reacts requires one mole of HCl. So if you use 19 mmol of sodium benzoate and 24 mmol of HCl then sodium benzoate would be your limiting reagent.

Calculating Molar Equivalents

Before converting moles to molar equivalents, you first need to determine your limiting reagent. Consider the example described above where sodium benzoate (19 mmol) is the limiting reagent and your other reagent is HCl (24 mmol). To calculate molar equivalents for each reagent, divide the moles of that reagent by the moles of the limiting reagent:

$$\text{molar equivalents of sodium benzoate} = \frac{19\ \text{mmol}}{19\ \text{mmol}} = 1.0$$

$$\text{molar equivalents of HCl} = \frac{24\ \text{mmol}}{19\ \text{mmol}} = 1.3$$

Note that the molar equivalency of sodium benzoate is 1. This is because sodium benzoate is the limiting reagent. Any reagents used in excess will have a molar equivalency greater than one. (Only a catalyst can have a molar equivalency of less than one.)

Calculating Theoretical Yield

Before calculating theoretical yield, you first need to determine your limiting reagent and identify the major product of the reaction. Consider the example described above where sodium benzoate (19 mmol) is the limiting reagent and your other reagent is HCl (24 mmol). In this example, the product is benzoic acid. In this example sodium benzoate reacts to form benzoic acid in a one-to-one ratio. So that means theoretically, 19 mmol of sodium benzoate should produce 19 mmol of benzoic acid. Next, you need to lookup the molecular weight of the product (it is 122.12 g/mol). Finally, all you need to do is convert moles to grams to get your theoretical yield:

$$\frac{122.12\ \text{mg}}{\text{mmol}}\ \text{X}\ 19\ \text{mmol} = 2{,}300\ \text{mg} = 2.3\ \text{g}$$

Calculating Percent Yield

Before calculating percent yield, you must have already calculated your theoretical yield. Also, you must have weighed your final product after it has completely dried. Let's consider the example above where the theoretical yield of benzoic acid was determined to 2.32 g. Pretend you isolated benzoic acid, dried it, and determined the final weight to be 2.03 g. Your percent yield would then be calculated by dividing the final weight by the theoretical yield and multiply by 100%:

$$\frac{2.03\ \text{g}}{2.32\ \text{g}}\ \text{X}\ 100\% = 87.5\%$$

Significant Figures and Calculations

As scientists you are required to report all final observations and calculated values with the correct number of significant figures. (Please review rules for preserving them.) In practice, perform all calculations with more digits than are significant (two decimal places is sufficient) and only round the very last number you report. Do not round intermediate values in the middle of your calculations, as this can create a rounding error.