

Organic Chemistry Calculations

There are three basic units for measurement in the organic laboratory – mass, volume, and number, measured in moles. Most of the other types of measurements are combinations of them, including density, molecular weight, molarity, and percent composition. Percent yield and percent recovery are ways to calculate the success of an experiment or isolation of a natural product.

Mass, Volume, and Density

Mass: Mass is a measurement of the amount of matter in a sample; fundamentally, it is a measurement of how much influence gravity has on the sample. In the metric system, mass is measured in grams (g). Mass is determined in the lab by using an electronic scale; the scales that we will use are accurate to 0.001 g.

In the metric system, units can be adjusted to accommodate different sizes. One gram (g) equals 1000 milligrams (mg). You can change grams to milligrams by multiplying by 1000, or milligrams to grams by dividing by 1000. In the equations below, substitute the number of milligrams (in the first equation) or grams (in the second equation) that you want to convert. (Notice that this is equivalent to moving the decimal point three places in the appropriate direction.) You should also check your answer logically – if you are going to a smaller unit (mg), you should have more of them, while if you are going to a larger unit (g), there should be fewer of them.

$10 \text{ mg} \times \frac{1 \text{ g}}{1000 \text{ mg}} = 0.01 \text{ g}$	$0.01 \text{ g} \times \frac{1000 \text{ mg}}{1 \text{ g}} = 10 \text{ mg}$
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The scales that we use measure in grams, but in this class it will be most convenient to work with milligrams when writing masses to avoid lots of decimals, so you will become very familiar with this conversion. If you have more than 1000 mg, convert it to grams; if you have less than 1.0 g, convert it to milligrams.

Volume: Volume is a measurement of how much space a sample occupies. In the metric system, volume is measured in liters (L). In the lab, we can measure volume by using a graduated cylinder, graduated pipet, or a labeled syringe. Volume can also be estimated by using the markings on a beaker, conical vial, or plastic pipet.

Liters can also change scale. One liter (L) equals 1000 milliliters (ml). You can convert liters to milliliters by multiplying by 1000, or milliliters to liters by dividing by 1000. Again, check your answer logically by looking at the size of unit you are going to and whether you should expect to have more or less of them. We will use milliliters much more often than liters in this class, so this conversion won't be as common.

$10 \text{ ml} \times \frac{1 \text{ L}}{1000 \text{ ml}} = 0.01 \text{ L}$	$0.01 \text{ L} \times \frac{1000 \text{ ml}}{1 \text{ L}} = 10 \text{ ml}$
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Density: Mass and volume are related by density. The density of a substance is how much mass there is in a sample compared to how much space it takes up. Lead has a high density (lots of mass in a small amount of space) while feathers have a low density (not much mass in lots of space). Density is given in grams per milliliter (g/ml), and it is a characteristic of a substance, usually in its liquid form.

Density can be determined experimentally by weighing out a known volume of a material. For example, you could put a graduated cylinder on a scale, zero it out, and then add 1 ml of a substance, and you will have the g/ml of that substance. If you did this for water, it would be 1.0 g/ml. Most organic liquids have densities similar to water, but they may be somewhat less dense (such as 0.86 g/ml, for example) or more dense (such as 1.21 g/ml).

In practice, we will look up densities of a substance in a catalog. The one that we will use is called the Aldrich Catalogue, which is published by the Sigma-Aldrich Chemical Company. This company wisely includes physical data along with prices in their catalogue, then gives it out to prospective clients for free, making it a valuable resource. The only difficulty is that you will need to learn to distinguish between multiple entries for a given compound, such as those of differing purity or those containing isotopes, which have different prices. The density is the number that follows a “d”.

Using the density of a substance, you can determine the mass of a given volume, or the volume of a given mass. This will be useful to us when working with liquids, which are often measured by volume. You can convert volume to mass by multiplying by the density, or mass to volume by dividing by the density. You can also check this logically by considering if the density is below or above 1.0. If it is above 1.0, then the mass should be the larger number. If it is lower than 1.0, then volume should be the larger number.

$10 \text{ ml} \times \frac{1.2 \text{ g}}{\text{ml}} = 12 \text{ g}$	$10 \text{ g} \times \frac{\text{ml}}{1.2 \text{ g}} = 8.3 \text{ ml}$
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Moles and Molecular Weight

Moles: The unit which measures the number of atoms or molecules in a sample is the mole (mol). Since atoms and molecules are incredibly small, the number of atoms or molecules in a reasonable sample is enormous, and 1 mole is a very large number: 6.02×10^{23} (called Avagadro’s number). A mole is like a dozen – it is just a word that represents a number, like a dozen means 12. If you have two dozen eggs, that means you have 24 eggs; likewise, if you have two moles of carbon, you have 12.04×10^{23} atoms of carbon.

Moles can be scaled just like grams or liters. One mole (mol) equals 1000 millimoles (mmol). To convert moles to millimoles, multiply by 1000; to convert millimoles to moles, divide by 1000. For the amounts we are working with, millimoles will be easier to use, so you will use this conversion a lot.

$10 \text{ mmol} \times \frac{1 \text{ mol}}{1000 \text{ mmol}} = 0.01 \text{ mol}$	$0.01 \text{ mol} \times \frac{1000 \text{ mmol}}{1 \text{ mol}} = 10 \text{ mmol}$
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Molecular weight: There is no way to directly measure the number of atoms or molecules in a sample – they are way too small to count! In order to find out how many moles of atoms or molecules are present, we must obtain the mass of the sample, convert it to moles using the molecular weight (MW) of the compound. The molecular weight is given in units of grams per mole – the number of grams in one mole of the compound.

To convert moles to grams, multiply by the molecular weight; to convert grams to moles, divide by the molecular weight. Notice that since molecular weight is a ratio, the molecular weight of a compound may be given as 100 g/mol or 100 mg/mmol. If you have milligram and you want millimoles (or vice versa), you can just use the molecular weight without changing it. However, if you have milligrams and want moles, you will have to divide by 1000.

$0.1 \text{ mol} \times \frac{100 \text{ g}}{\text{mol}} = 10 \text{ g}$	$10 \text{ g} \times \frac{\text{mol}}{100 \text{ g}} = 0.1 \text{ mol}$
$0.1 \text{ mmol} \times \frac{100 \text{ mg}}{\text{mmol}} = 10 \text{ mg}$	$10 \text{ mg} \times \frac{\text{mmol}}{100 \text{ mg}} = 0.1 \text{ mmol}$

To obtain the molecular weight for a particular compound, we use the molecular formula for the compound and the atomic weight of each element, which has been determined experimentally and is given on the Periodic Table of Elements. Add up the atomic weights of each atom in the molecule. Use two decimals (three for hydrogen), and don't round until you have finished your calculation.

$$\text{MW} = (\text{number of C} \times 12.01 \text{ g/mol}) + (\text{number of H's} \times 1.007 \text{ g/mol}) + \text{etc.}$$

Molarity and Percent Composition of Solutions

Most substances don't react with each other when both are in solid form. The molecules aren't moving much, so they don't bump into each other and don't react. In order to get solids to react with each other, we need to dissolve them in a liquid. Many reagents are added to a reaction already in solution. Therefore, we need a way to know how many moles of the reagent are present in a certain volume of the solution. The two most common ways to define the concentration of a solution in organic chemistry are by molarity and % composition by mass.

Molarity: Molarity is measured in moles per liter of solution. If a solution has two moles of the compound for every liter of solution, it is said to be 2 molar, or 2M. These kinds of solutions take some calculations to prepare (you have to figure out a mass 2 moles of the reagent so you can weigh it out), but are very easy to use once they are prepared. To find out how many moles of the reagent are in a certain volume of solution, simply multiply the volume by the molarity. To find out how much of a solution you need to have a certain number of moles, divide by molarity.

$0.1 \text{ L} \times \frac{2 \text{ mol}}{\text{L}} = 0.2 \text{ mol}$	$0.2 \text{ mol} \times \frac{\text{L}}{2 \text{ mol}} = 0.1 \text{ L}$
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Percent composition: Percent composition solutions are measured in grams of compound per 100 grams of solution. So if a solution has 20 grams of the compound in every 100 grams of solution, it is said to be a 20% solution. These kinds of solutions are easy to prepare – just take 20 grams of the compound and add the solvent until the total reaches 100 g. They are more difficult to work with, however, because you have to do several calculations to find out how many moles are present.

If you have the volume of the solution and its density, you can figure out the mass of the solution, using density as above. Then, you can use the mass of the solution and the percent composition to figure out the mass of the dissolved compound. You can then use the mass of the compound and its molecular weight to determine the moles of the compound. To go from moles of the compound to volume of the solution, do these steps in reverse.

$20 \text{ g solution} \times \frac{20}{100} = 5 \text{ g solute}$	$5 \text{ g solute} \times \frac{100}{20} = 20 \text{ g solution}$
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Molar Equivalents

Knowing the number of moles is important when running a reaction involving two different substances. If you simply measured out 1 gram of each of them, you would not have the same number of molecules. Likewise, if you measured out 1 ml of each of them, the number of molecules still wouldn't match up. Instead, you need to have equal numbers of moles.

For example, if you have a dozen fried eggs and a dozen pieces of toast, the pile of eggs won't have the same mass as the pile of toast, or take up the same space, but you can match them up and have a dozen plates of eggs and toast. In the same way, if you have 2 moles of compound A and 2 moles of compound B, you have the same number of molecules of A and B, but they won't have the same mass or volume.

We will use molar equivalents (eq) to compare the number of moles of different compounds. In the egg and toast example above, the ratio is 1 to 1, so we would say that there is 1 equivalent of eggs and 1 equivalent of toast. On the other hand, if you have 3 moles of compound A and 6 moles of compound B, then you have 1 equivalent of A and 2 equivalents of B; alternatively, you could say that you have 0.5 eq of A and 1 eq of B – you can choose which you want to have equal to 1 eq. This is very useful when planning reactions, since we will want to plan out the ratio of molecules in the reaction mixture.

$\frac{6 \text{ mol B}}{3 \text{ mol A}} = 2 \text{ eq B}$	$\frac{3 \text{ mol A}}{3 \text{ mol B}} = 1 \text{ eq A}$
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Reaction Tables

When it is time to run a reaction, all of these calculations come together.

The calculations begin with the organic compound that will be used as the limiting reagent. The limiting reagent is the compound that limits the amount of product that can be formed – in other words, it is what you will run out of first. It is important to plan which compound this will be – it is usually the largest organic compound in the reaction. This is the easiest compound to define as having one equivalent – then you can look at the molar equivalents of everything else in comparison to it.

Once you have chosen a limiting reagent, an amount of this compound is chosen, and then its moles are calculated. You must then decide how many equivalents of each of the other reagents to use. You can think of this as the recipe for this reaction - what molar ratio of each reagent do you want to use compared to the limiting reagent? The following are some reasons for including more or less than 1 equivalent of a reagent:

1. It is common to use a slight excess of all reagents except the limiting reagent, just to be on the safe side. This ensures that slight errors in measurement won't affect the outcome of the reaction by making you run short of something you didn't plan to.
2. The coefficients of the reaction must be taken into account. For example, if the reaction requires 2 moles of a reagent for every mole of the limiting reagent, then you should have at least 2 equivalents of that reagent.
3. If a reagent is unusually reactive or volatile (evaporates easily), you will probably want to use more than one equivalent in case some of it has already reacted or it evaporates as the reaction occurs.
4. If you are performing a two step reaction, it is important to set the starting material of the second reaction as the limiting reagent, and have extra of the starting materials for the first reaction. That way if the first reaction doesn't go all the way, you will still have enough for the second reaction to proceed.
5. If the equilibrium of a reaction is near 1.0, you can use up to 10 equivalents or more of one reagent in order to use up the starting material and cause more product to form.
6. Catalysts and other reagents that are not consumed by the reaction should be present in amounts smaller than one equivalent. They don't run out, so even with less than one equivalent, they won't limit amount of product that will be formed.

Once you have decided on the molar equivalents for each reagent, the amounts of these reagents that you will need to measure out can be calculated. For solids, this is usually mass. For liquids or solutions, this is usually volume.

It is easiest to keep track of your data in a table which includes all reagents as well as the predicted product of the reaction. A typical table includes mass, density, volume, molecular weight (or molarity for a solution), moles, and molar equivalents.

Percent Yield and Percent Recovery

Percent yield: When you run a reaction and recover the product, you will need to find out how much of the material you started with was converted into the product you have in your hand.

This is done by first calculating the total expected amount if all of the limiting reagent was converted to product – this is called the theoretical yield. Look at the limiting reagent to figure out how many moles there were. The theoretical yield of product will have the same number of moles as the limiting reagent. You can then figure out how many grams of product to expect.

Comparing the actual yield to the theoretical yield gives the % yield. Take the actual amount that you measured (in grams) and divide it by the theoretical yield, or how much you could have gotten if everything had gone perfectly.

$$\text{percent yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\%$$

In practice, very few reactions achieve 100% yields. Some of the product is usually lost during the procedures needed to separate it from the reaction mixture. Also, few reactions go to 100% completion in the first place. Some starting materials are usually present at the end of the reaction.

If you obtain more product than the theoretical yield, this is an indication that something has gone wrong, since you can't get more than you started with! The most likely reasons are that either you measured incorrectly, or the product is still contaminated with some other compound such as water or solvent.

Percent Recovery: In some experiments we will perform a chemical reaction in which one compound is converted to another. In other experiments we will simply isolate an existing compound from where they are found in nature (beta carotene from spinach leaves, for example).

In this second kind of experiment, a % yield cannot be calculated, because no reaction takes place – there is no starting material or product, just a compound which has been separated from a mixture. Instead, we simply calculate a % recovery – the amount of the desired compound compared to the amount of the original material it was taken out of, both measured in grams.

$$\text{percent recovery} = \frac{\text{amount recovered}}{\text{starting amount}} \times 100\%$$