A Step-by-step Guide to Calculating Limiting Reagent, Theoretical Yield, and Percent Yield

Yield calculations are common in chemistry. I've helped many frustrated students with these calculations in the past, so I developed this guide to help. Calculating percent yield actually involves a series of short calculations. Follow this step-by-step guide and you will be able to calculate limiting reagent, theoretical yield, and percent yield.

1. Write a balanced equation for the reaction

2. Calculate the molecular weight of each reactant and product

3. Convert all amounts of reactants and products into moles

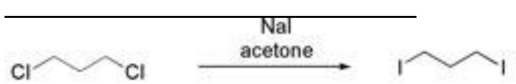
4. Figure out the limiting reagent

5. Calculate the theoretical yield

6. Calculate the percentage yield

1. Write a balanced equation for the reaction: To figure out percentage yield you need to know the correct ratio of each of the reactants and products of interest (this is called stoichiometry).

• Many times reactions are not written in balanced form. Make sure you are looking at a balanced equation before trying to do any yield calculations.



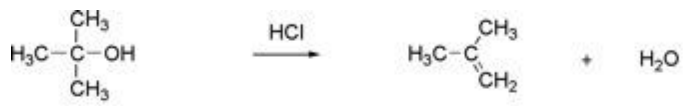
equation 1
not balanced

equation 2
balanced

• Be sure you can distinguish between reagents, solvents, and catalysts. Any species that is not consumed in the reaction doesn't figure into the yield calculation. See the next example.

Example:

Note that in the examples above HCl functions in different ways. In **equation 3**, HCl is a catalyst, and does not get consumed in the reaction. However, in **equation 4**, HCl is consumed and is a reagent.

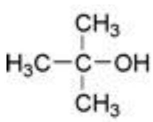


equation 3
HCl is a catalyst

equation 4
HCl is a reagent

<u>2. Calculate the molecular weight of each reactant and product:</u> You will need to know these numbers to do yield calculations.

• To calculate the molecular weight of a molecule, simply add up the masses of the individual atoms.
Example:



This molecule contains 4-carbons, 10 hydrogens, and 1 oxygen

weight of carbon atoms = 4 X 12.01 g = 48.04 g
weight of hydrogen atoms = 10 X 1.01 g = 10.10 g
weight of oxygen atom = 1 X 16.00 g = 16.00 g

molecular weight (MW) = 74.14 g

<u>3. Convert all amounts of reactants and products into moles:</u> Usually reactants are measured out by volume or mass. You need to know these quantities in terms of moles to do yield calculations. The conversion of volume and mass into number of moles can be done using the density and molecular weight of the material

• Mass can be converted to moles using molecular weight. Be sure to include all units in your calculations. It will help you to avoid errors. By insuring that the mass units cancel in the calculation you can be sure you have the calculation setup properly.
Example:

Consider the reaction in **equation 3** above. Suppose you used 25.0 g of the reactant $(CH_3)_3COH$. To convert grams to moles use the molecular weight. So how do you know whether to multiply or divide by the molecular weight? Answer: look at the units, grams should cancel in the calculation, leaving an answer that has units of moles. This is illustrated below.

$$\underbrace{\frac{25.0\ \cancel{g\ (CH_3)_3COH}}{1}}_{\text{quantity of compound in grams}} \times \underbrace{\frac{1\ mol\ (CH_3)_3COH}{74.14\ \cancel{g\ (CH_3)_3COH}}}_{\text{molecular weight of the compound}} = \underbrace{0.337\ mol\ (CH_3)_3COH}_{\text{quantity of compound in moles}}$$

• To convert volume to moles, first convert to mass using density, then convert to moles using molecular weight. Again, be sure to include all units in your calculations. It will help you to avoid errors.
Example:

Again consider the reaction in **equation 3** above. Suppose you used 30.0 mL of the reactant $(CH_3)_3COH$. First convert this volume into mass using density (g/mL), then convert grams to moles using the molecular weight. Again, include units and set up your calculation so that milliliters and grams cancel in the calculation leaving an answer that has units of moles. This is illustrated below.

$$\frac{30.0\ \cancel{\mathrm{mL\ (CH_3)_3COH}}}{1} \times \frac{0.775\ \cancel{\mathrm{g\ (CH_3)_3COH}}}{1\ \cancel{\mathrm{mL\ (CH_3)_3COH}}} \times \frac{1\ \mathrm{mol\ (CH_3)_3COH}}{74.14\ \cancel{\mathrm{g\ (CH_3)_3COH}}} = 0.314\ \mathrm{mol\ (CH_3)_3COH}$$

quantity of compound in milliliters	density of the compound	molecular weight of the compound	quantity of compound in moles

• If you use a certain volume of a solution of known concentration, you can calculate moles from these two quantities. Again, set up an equation with units so that everything but moles cancels out. See the example below.

$$\frac{20.0\ \cancel{\mathrm{mL\ 12M\ HCl}}}{1} \times \frac{1\ \cancel{\mathrm{L\ 12M\ HCl}}}{1000\ \cancel{\mathrm{mL\ 12M\ HCl}}} \times \frac{12\ \mathrm{mol\ HCl}}{1\ \cancel{\mathrm{L\ 12M\ HCl}}} = 0.24\ \mathrm{mol\ HCl}$$

quantity of solution in milliliters	converting millilieters into liters	molarity of solution	quantity of compound in moles

4. Figure out the limiting reagent: Now take inventory of the number of moles of each reactant present and look at the balanced equation. If the reaction takes place consuming the reactants as indicated by the equation, which reactant will run out first? This is the limiting reagent

1 bun + 2 beef patties ⟶ 1 Big Mac

Example:

This time let's consider a chemistry reaction in the balanced **equation 2** from above. If we started with 10 mol of $ClCH_2CH_2CH_2Cl$ and 12 mol of NaI, which reagent will get used up first?

The answer is that NaI is limiting. You have enough $ClCH_2CH_2CH_2Cl$ to make 10 mol of $ICH_2CH_2CH_2I$, but you can only make 6 mol of this product with the NaI that you started with (because you use two NaI molecules on every $ClCH_2CH_2CH_2Cl$). Therefore, NaI runs out first and it is the limiting reagent.

10 mol 12 mol

5. Calculate the theoretical yield: The theoretical yield is the yield you would get if the reaction worked perfectly. That is, if every molecule reacted exactly as it was supposed to, and no material was lost at any stage. The theoretical yield is based on the moles of limiting reagent you started with. Look at the number of moles of limiting reagent and look at the balanced equation. If the reaction takes place consuming the limiting reagent as indicated by the equation, how much product will be produced? This is the theoretical yield.

Example:

Let's consider a simple example first, **equation 3** from above. In this example, there is only one reactant $(CH_3)_3COH$, so this is the limiting reagent (remember HCl is a catalyst in this reaction). If we started with 1 mol of $(CH_3)_3COH$, how many moles of $(CH_3)_2C{=}CH_2$ would we expect for a theoretical yield?

The answer is theoretical yield = 1 mol. The stoichiometry of this reaction is such that every molecule of the limiting reagent gives one molecule of $(CH_3)_2C{=}CH_2$.

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

$$= \frac{0.55\ \cancel{\text{mol}}}{1.0\ \cancel{\text{mol}}} \times 100 = 55\ \%$$

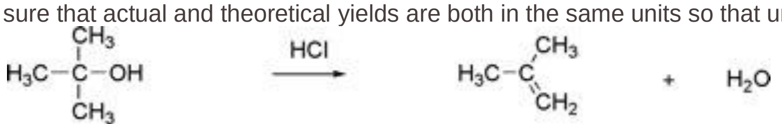
Example:

Now let's consider an example from before. In part 4 above we determined that if we started with 10 mol of $ClCH_2CH_2CH_2Cl$ and 12 mol of NaI in the reaction below that NaI was the limiting reagent. Under these conditions, what is the theoretical yield of $ICH_2CH_2CH_2I$?

The answer is theoretical yield = 6 mol. It takes two molecules of NaI to make one molecule of $ICH_2CH_2CH_2I$.

10 mol 12 mol

<u>6. Calculate the percentage yield:</u> The percent yield is simply the actual yield divided by theoretical yield multiplied by 100. Actual yield is the amount of product you actually got while theoretical is the maximum possible yield. Be sure that actual and theoretical yields are both in the same units so that units cancel in the calculation.



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

$$= \frac{0.55\,\cancel{\text{mol}}}{1.0\,\cancel{\text{mol}}} \times 100 = 55\ \%$$