Mole Tables

When setting up a reaction, organic chemists use a mole table to figure out the mass and volume of reagents needed based on the reaction stoichiometry. The mole table is a convenient way to organize all the information needed to determine the limiting reagent and theoretical yield, which are then used to calculate percent yield. The percent yield tells the chemist how efficient a reaction is and must be included in published accounts of reactions.

<u>How to Find Moles</u>

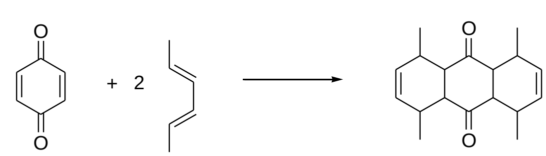
Solids – if you are given the grams of a solid reagent, finding moles is as simple as dividing by the molar mass (a.k.a. molecular weight (MW) or formula weight (FW))

Liquids – it is more convenient to measure liquids as volumes, rather than try to weigh them on a balance. Therefore, to find moles of a liquid, we first find grams by multiplying the milliliters of liquid measured by its density, then divide the grams of liquid by the molar mass of the compound.

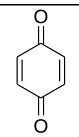
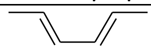
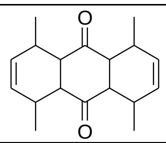
Solutions – if the liquid is not a pure reagent, but is instead a solution having more than one component, your calculations must take that into account. If the concentration of the solution is given as molarity, moles can be found my multiplying molarity by the volume of reagent in liters. If the concentration of reagent is given as a mass percent, first the grams of the entire solution (reagent + solvent) are found by multiplying volume by the density of the solution; next, the grams of reagent are found my multiplying the total grams by the percent reagent as a decimal (ex. – if 30% by mass, multiply by 0.30); finally, divide the grams of reagent by molar mass to find the moles.

<u>Setting up a Mole Table</u>

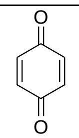
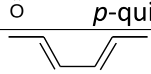
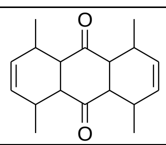
The mole table organizes all the information needed to find moles of the various reagents. Minimum, it will include columns for the name and structure of the reagent, mass, molar mass, and moles. If reagents are liquids or solutions, columns for volume, density, and concentration should be added as needed. Solvents, extraction liquids, and drying agents do not need to be included in the mole table. Only reagents that take part in the mechanism are included. Catalysts – reagents that are used at the beginning of a mechanism and are regenerated by the end of the mechanism – can be included in the mole table, but cannot be the limiting reagent and therefore should not be included in those calculations.



Suppose we are carrying out the above reaction in laboratory class. The mass of solids and the volume of liquids to be used would be given in the procedure; the molar masses and densities can be looked up in a reference book or MSDS. (If you do not know the name of a product, you can still find its mass because molecular formula can always be deduced from a structure.) Before you begin any calculations, the mole table will look like this:

	molar mass (g/mol)	mass (g)	volume (mL)	density (g/mL)	moles
 *p*-quinone	108.09	2.50	-	-	
 *(2E,4E)*-2,4-hexadiene	82.15		5.00	0.720	
	273.39		-	-	

Using the procedures above, you will calculate moles for each reagent. In this case, p-quinone is a solid, and 2,4-hexadiene is a pure liquid. Once the preliminary calculations are done, the table should look like the one below. Try the calculations for yourself.

	molar mass (g/mol)	mass (g)	volume (mL)	density (g/mL)	moles
 *p*-quinone	108.09	2.50	-	-	0.0231
 *(2E,4E)*-2,4-hexadiene	82.15	3.60	5.00	0.720	0.0438
	273.39		-	-	

<u>Calculating Limiting Reagent</u>

The limiting reagent is the reagent that will be used up first and which limits the amount of product that can be formed. If the reagents react with 1:1 stoichiometry, the limiting reagent is simply the reagent with fewer moles. However, if reagents do not react in a 1:1 ratio, as in our sample problem above, calculations must be done to find the limiting reagent. The limiting reagent is not necessarily the reagent with fewer moles.

Using the molar ratio, calculate the theoretical moles of product that could be produced from the moles of each reagent. The molar ratio is based on the coefficients in a balanced equation. For a more detailed explanation see your CHM 111 text.

$$\frac{0.0231 \text{ mol quinone}}{} \times \frac{1 \text{ mol product}}{1 \text{ mol quinone}} = \frac{0.0231 \text{ mol product}}{}$$

$$\frac{0.0438 \text{ mol diene}}{} \times \frac{1 \text{ mol product}}{2 \text{ mol diene}} = \frac{0.0219 \text{ mol product}}{}$$

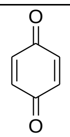
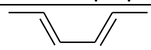
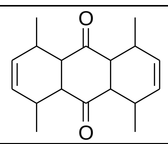
The reagent that can produce the least theoretical moles of product is the limiting reagent. In this case, 2,4-hexadiene is the limiting reagent, even though we are using more moles of 2,4-hexadiene in the reaction than we have of quinone.

<u>Calculating Theoretical Yeild and % Yield</u>

Once you have found the limiting reagent and determined the maximum theoretical moles of product, you multiply it by the molar mass of the product to get the theoretical yield. The theoretical yield should always be given in grams and calculated before class. For the example reaction:

$$\text{Theoretical Yield} = \frac{0.0219\ \text{mol product}}{} \times \frac{273.39\ \text{g product}}{1\ \text{mol product}} = 5.99\ \text{g}$$

Your finalized mole table would look like this:

	molar mass (g/mol)	mass (g)	volume (mL)	density (g/mL)	moles
 p-quinone	108.09	2.50	-	-	0.0231
 (2E,4E)-2,4-hexadiene	82.15	3.60	5.00	0.720	0.0438
	273.39	5.99 (theoretical)	-	-	0.0219

At the end of your experiment, you will weigh your product and divide by the theoretical yield to find the percent yield. If your actual yield in this reaction was 4.25 g, the calculations would be as follows.

$$\text{Percent Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100\% = \frac{4.25\text{g}}{5.99\text{g}} \times 100\% = 71.0\%$$

In your discussion you should mention your percent yield and give possible reasons for an unusually low yield. If your actual yield is higher than your theoretical yield, you know it must contain solvent or other contaminants and you should speculate on what they might be.