

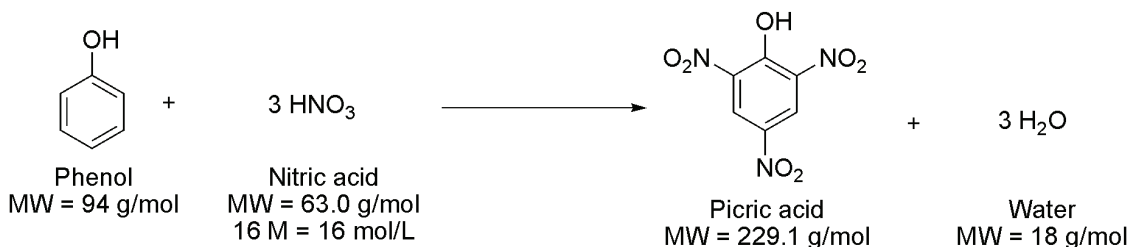
## Review of Calculations for Organic Reactions (#1a)

In your experiments the quantities of many reactants are given in mass or volume, though chemicals react in mole ratios, because it is not possible to measure a quantity in moles easily. You will have to convert mass or volume (mass = volume x density) to moles before beginning an experiment. You will also have to recognize stoichiometric relationships between reactants and products, which is based on mole ratio, in order to be able to calculate the theoretical yield of product you expect to isolate. You will apply the knowledge from this session to complete the theoretical yield calculation in your prelab reports and postlab reports.

In this lab you are expected to be able to differentiate between a limiting reagent and excess reagents, solvents and catalysts which are crucial for the reaction to occur and go to completion. A **limiting reagent** is a reactant that has the lowest number of moles of all reactants in the chemical reaction and once it is completely consumed the reaction terminates. An excess reagent is a reactant that has a higher number of moles and therefore is not used up when a reaction goes to completion. Solvents and catalysts are not involved in the determination of limiting reagent.

An example of calculations that you will be expected to perform is shown using the reaction of phenol with nitric acid. Preparation of picric acid requires the nitration of phenol. Given 5.00 grams of phenol and 15.0 mL concentrated nitric acid (15.9 M), one can determine the **MAXIMUM** theoretical amount of picric acid formed. The first step in this process is to determine which reagent is the **limiting reagent**. To do this you simply calculate the number of moles of each available reagent. When calculating limiting reagents, there are a few important details. For instance, you should realize that if you use a reagent as a solvent in a reaction, it is never the limiting reagent. Also if you are using a reagent that is a catalyst, it will **not** be the limiting reagent. Another very important detail is the stoichiometry of a reaction. For instance, in the reaction shown you will notice that 3 moles of nitric acid are used for every one mole of phenol and you only form one mole of product.

From the calculations above, notice that there is less phenol than nitric acid. Thus you can only form 0.0531 moles of picric acid. So once all the phenol has been used up in the formation of the picric acid, there will be some nitric acid left which will not have any substrate to react with and



$$5.00 \text{ g phenol} \times \frac{1 \text{ mol phenol}}{94 \text{ g phenol}} \times \frac{1 \text{ mol picric acid}}{1 \text{ mol phenol}} = 0.05 \text{ moles picric acid}$$

$$15 \text{ mL HNO}_3 \times \frac{16 \text{ mmol HNO}_3}{1 \text{ mL HNO}_3} \times \frac{1 \text{ mol HNO}_3}{1000 \text{ mmol HNO}_3} \times \frac{1 \text{ mol picric acid}}{3 \text{ moles HNO}_3} = 0.08 \text{ moles picric acid}$$

will simply be excess. Now that you know which reagent is the limiting reagent, you can determine the amount of product that could **theoretically** be formed. Therefore 0.0531 moles X 229.1 g/mol = 12.2 g of picric acid can be formed. It is *very* rare to obtain the **theoretical yield**, so it is desirable to calculate a **percentage yield** based on the theoretical yield.

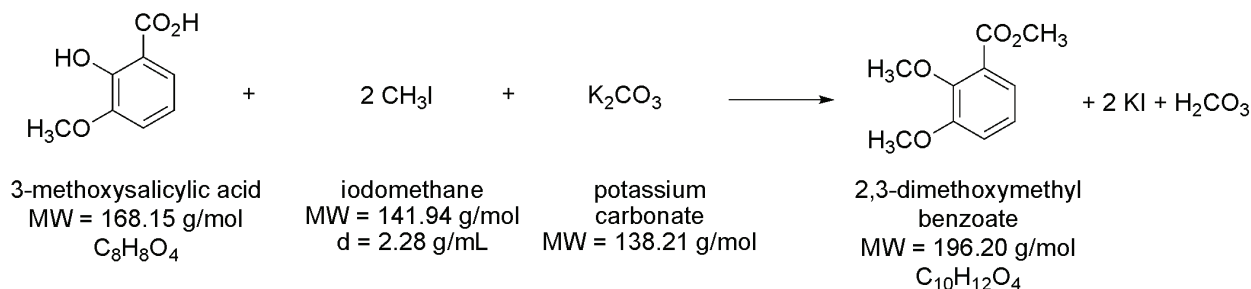
$$\text{Percentage Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100\%$$

From this information, suppose the **actual yield** that a student obtained is 10.4 g of picric acid. Using the above equation [(10.4/12.2) X 100% = 85%] you see that the student obtained 85% of the theoretical amount possible.

### Postlab

You should complete the following assignment **in your lab notebook with your postlab reports**. Include your name, the title of the assignment, and your section number (1 pt) on each page. Include a purpose statement describing the objectives of the assignment (2 pts).

1. Using the reaction shown below, calculate the percent yield obtained by a student when reacting 5.0 g of 3-methoxysalicylic acid with 3.9 mL of iodomethane in the presence of 10.3 g of potassium carbonate and obtaining 4.5 g of product, 2,3-dimethoxymethyl benzoate. You should determine which of the three reactants is the limiting reagent and the theoretical yield first.



2. Using the reaction shown below, calculate the number of milliliters of bromine required to react completely with 5 g of 1,2-dimethoxybenzene.

