Calculating Theoretical and Percent Yield

General Procedure

- 1) Balance the chemical equation
- 2) Convert the grams or milligrams of reactants to moles or millimoles.
- 3) Find the limiting reagent (the reactant that limits the reaction to produce the least amount of product)
- 4) Calculate the moles of product expected if the reaction goes to 100%.
- 5) Calculate the grams of product from the moles of product. This is the theoretical yield in grams.
- 6) Calculate the percent yield: % Yield = $\frac{\text{Actual yield}}{\text{Theoretical Yield}} \times 100\%$

Example

Suppose the above reaction uses 300. mg of dibromide and 247 mg of KOH. The reaction yielded 115 mg of diphenylacetylene.

- 1) The equation written above is already balanced.
- 2) Calculate the of mmol of each reactant:

Dibromide:
$$300. \text{ mg} \times \frac{1 \text{ mmol}}{340 \text{ mg}} = 0.882 \text{ mmol}$$

Potassium Hydroxide: 247 mg
$$\times \frac{1 \text{ mmol}}{56 \text{ mg}} = 4.41 \text{ mmol}$$

3) Determine the limiting reagent:

Dibromide: 0.882 mmol
$$\times \frac{1 \text{ mmol product}}{1 \text{ mmol dibromide}} = 0.882 \text{ mmol product (limiting reagent)}$$

Potassium Hydroxide: 4.41 mmol
$$\times \frac{1 \text{ mmol product}}{2 \text{ mmol KOH}} = 2.21 \text{ mmol product (excess reagent)}$$

4) Based on the limiting reagent calculation, if the reaction goes to 100% completion, the maximum amount of product that can be formed is 0.882 mmol.

5) Theoretical Yield:
$$0.882 \text{ mmol} \times \frac{178 \text{ mg}}{1 \text{ mmol}} = 157 \text{ mg}$$

6) **Percent Yield:**
$$\frac{115 \text{ mg}}{157 \text{ mg}} \times 100\% = 73.2 \% \text{ yield}$$