Percent Yield Calculations

Percent yield calculations are one of the most commonly used calculations in organic chemistry lab. Unfortunately the calculations are also one of the most common areas where students make mistakes. Understanding how to routinely and accurately carry out percent yield calculations will bolster understanding of the chemistry behind the calculation and simultaneously help improve grades.

The amount of product which can form from each starting material must be calculated. This defines what is the limiting reagent and allows the percent yield to be determined. The calculations necessary to determine the Percent Yield calculations can be broken down into 3 simple steps.

**Necessary Steps**
1. Determine the amount of product (usually in grams) which can form from EACH starting material. A separate calculation must be done for each starting material. Catalysts and solvents are not stoichiometric reagents and cannot be converted into product.
2. The reactant which will produce the smallest amount of the product is the limiting reagent. The limiting reagent is the starting material which will be depleted first. The amount of product formed from the limiting reagent is the theoretical maximum amount of product which can form.
3. Determine the percent yield of the reaction by dividing actual grams of product formed by the theoretical maximum amount of product possible X 100%.

Dimensional analysis is very helpful in arriving at the correct answer. **Include all units and identifiers.** *Often when a student is unsure how to proceed while solving a problem, a close examination of the units will direct the correct next multiplication or division.*

**Reminders**
* **NEAT MATERIALS**, are liquids without solvent. Density is used to convert a volume of a neat liquid into mass.
* Molecular weight is used to convert from mass to moles.
* Stoichiometry is used to convert from moles of reactants to moles product.

\[
\text{Volume Reactant (mL or L)} \quad \text{Mass Reactant (g)} \quad \text{Moles Reactant (mol)} \quad \text{Reaction Stoichiometry} \quad \text{Moles Product (mol)} \quad \text{Molar Mass Product (g/mol)} \quad \text{Mass Product (g)}
\]

* If a **SOLUTION** (as opposed to a neat liquid) is used, then the concentration of that solution must be taken into account. The volume (in liters) of solution used can be multiplied by the molarity (M = moles/L) of the solution to determine moles of the active material in the solution.

\[
\text{Volume Solution (L)} \quad \text{Moles Reactant (mol)} \quad \text{Reaction Stoichiometry} \quad \text{Moles Product (mol)} \quad \text{Molar Mass Product (g/mol)} \quad \text{Mass Product (g)}
\]

* Keep track of all units.
* Be very aware of the stoichiometry of the reaction.
* All data provided may not have to be used to determine answer.
Practice problem 1. One material measured as a solid (g) one material as a neat liquid (mL).
2.897 g of maleic anhydride (MA) is reacted with 2.56 mL of cyclohexadiene (CHD) to produce 3.979 grams of the bicyclic product. What is the limiting reagent and what is the percent yield?

![Chemical structure](attachment:image.png)

<table>
<thead>
<tr>
<th>name</th>
<th>cyclohexadiene (CHD)</th>
<th>maleic anhydride (MA)</th>
<th>5,6-anhydride [2.2.2]bicyclo-2-octene</th>
</tr>
</thead>
<tbody>
<tr>
<td>density (g/ml)</td>
<td>0.8405</td>
<td>1.314</td>
<td></td>
</tr>
<tr>
<td>mol. Wt. (g/mol)</td>
<td>80.15</td>
<td>98.06</td>
<td>178.20</td>
</tr>
<tr>
<td>volume (mL)</td>
<td>2.56</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>mass (g)</td>
<td>-</td>
<td>2.897</td>
<td>3.979</td>
</tr>
</tbody>
</table>

**Step 1) Amount of product possible from each starting material**
From maleic anhydride (solid)
\[
\frac{2.897 \, g \, MA(g)}{98.06 \, g \, MA(g)} \times \frac{1 \, mole \, MA(mol)}{1 \, mole \, Product} \times \frac{178.20 \, grams \, product}{1 \, mole \, Product} = 5.265 \, grams \, Product
\]
From cyclohexadiene (neat liquid)
\[
\frac{2.56 \, mL \, CHD}{80.15 \, g \, CHD} \times \frac{0.8405 \, g \, CHD}{1 \, mL \, CHD} \times \frac{1 \, moles \, CHD}{1 \, mole \, CHD} \times \frac{178.20 \, grams \, product}{1 \, mole \, product} = 4.78 \, g \, Product
\]

**Step 2) Theoretical Maximum and Limiting Reagent**
Since 4.78 is smaller than 5.265, cyclohexadiene is the limiting reagent and 4.78 g is the theoretical maximum amount of product which can form. (note the significant figures)

**Step 3) Percent Yield.** Using knowledge of actual amount of product formed, calculate the % yield.
\[
\frac{Actual \, Mass \, Product \, Formed(g)}{Theoretical \, Maximum \, Mass \, Product(g)} \times 100\% = \% \, yield \, Product
\]
\[
\frac{3.979 \, g \, Product}{4.78 \, g \, product} \times 100\% = 83.2\% \, yield \, Product
\]

Practice Problem 2. One material measured as a solution (M) one as a neat liquid (g).
4.24 mL of 2-butanol is reacted with 10.2 mL of 6.0 M HCl to form 2.8798 grams of 2-chlorobutane. What is the limiting reagent and what is the percent yield.

![Chemical structure](attachment:image.png)

<table>
<thead>
<tr>
<th>name</th>
<th>2-butanol (BuOH)</th>
<th>Hydrochloric Acid (6.0 M)</th>
<th>2-chlorobutane</th>
<th>Water</th>
</tr>
</thead>
<tbody>
<tr>
<td>density (g/ml)</td>
<td>0.808</td>
<td>1.314</td>
<td></td>
<td>1.00</td>
</tr>
<tr>
<td>mol. Wt. (g/mol)</td>
<td>74.1</td>
<td>36.5</td>
<td>92.6</td>
<td>18.00</td>
</tr>
<tr>
<td>volume (mL)</td>
<td>4.24</td>
<td>10.2</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>mass (g)</td>
<td>-</td>
<td>-</td>
<td>2.8798</td>
<td></td>
</tr>
</tbody>
</table>
Step 1) Amount of product possible from each starting material

From 2-butanol (neat liquid)

\[
\frac{4.24 \text{ ml } \text{BuOH}}{1 \text{ ml } \text{BuOH}} \times \frac{0.808 \text{ g } \text{BuOH}}{74.1 \text{ g } \text{BuOH}} \times \frac{1 \text{ mole } \text{BuOH}}{1 \text{ mol } \text{BuOH}} \times \frac{92.6 \text{ g } \text{Prod}}{1 \text{ mol } \text{Prod}} = 4.28 \text{ grams Product}
\]

From hydrochloric acid (solution)

\[
\frac{10.2 \text{ ml } \text{HCl}}{1000 \text{ ml } \text{HCl}} \times \frac{1 \text{ L } \text{HCl}}{6.0 \text{ mol } \text{HCl}} \times \frac{1 \text{ mol } \text{Prod}}{1 \text{ mol } \text{HCl}} \times \frac{92.6 \text{ g } \text{Prod}}{1 \text{ mol } \text{Prod}} = 5.7 \text{ grams Product}
\]

Step 2) Theoretical Maximum and Limiting Reagent

Since 4.28 is less than 5.7, 2-butanol is the limiting reagent and the maximum theoretical amount of product which can form is 4.28 g.

Step 3) Percent Yield. Using knowledge of actual amount of product formed, calculate the % yield.

\[
\frac{\text{Actual Mass Product Formed (g)}}{\text{Theoretical Maximum Mass Product (g)}} \times 100\% = \text{yield Product}
\]

\[
\frac{2.8798 \text{ g } \text{Product}}{4.28 \text{ g } \text{product}} \times 100\% = 67.3\% \text{ yield} 
\]

Practice Problem 3. Non 1 : 1 stoichiometry. One is a neat liquid (mL) one a solution (M).

7.3 mL of neat methyl benzoate is reacted with 15.2 mL of 5.0 M bromobenzene in an excess of magnesium shavings and an acid work-up to produce triphenylmethanol. What is the limiting reagent, the theoretical maximum amount of product which can form, and the percent yield? (An excess of magnesium is used.)

![Chemical structure image]

<table>
<thead>
<tr>
<th>name</th>
<th>methyl benzoate (MB)</th>
<th>Bromobenzene (BrB)</th>
<th>triphenylmethanol</th>
</tr>
</thead>
<tbody>
<tr>
<td>density (g/ml)</td>
<td>1.09</td>
<td>1.50</td>
<td></td>
</tr>
<tr>
<td>mol. Wt. (g/mol)</td>
<td>136.1</td>
<td>157.02</td>
<td>260.3</td>
</tr>
<tr>
<td>volume (mL)</td>
<td>7.3</td>
<td>10.0</td>
<td></td>
</tr>
<tr>
<td>mass (g)</td>
<td>-</td>
<td>-</td>
<td>6.655</td>
</tr>
</tbody>
</table>

Step 1) Amount of product possible from each starting material

\[
\frac{7.3 \text{ ml } \text{MB}}{1 \text{ ml } \text{MB}} \times \frac{1.09 \text{ g } \text{MB}}{136.1 \text{ g } \text{MB}} \times \frac{1 \text{ mole } \text{MB}}{1 \text{ mol } \text{MB}} \times \frac{1 \text{ mol } \text{Prod}}{1 \text{ mol } \text{MB}} \times \frac{260.5 \text{ g } \text{Prod}}{1 \text{ mol } \text{prod}} = 15 \text{ g } \text{Prod}
\]

\[
\frac{15.2 \text{ ml } \text{BrB}}{1000 \text{ ml } \text{BrB}} \times \frac{1 \text{ L } \text{BrB}}{2 \text{ mol } \text{BrB}} \times \frac{5.0 \text{ mol } \text{BrBe}}{1 \text{ mol } \text{BrB}} \times \frac{1 \text{ mol } \text{Prod}}{2 \text{ mol } \text{BrB}} \times \frac{260.5 \text{ g } \text{Prod}}{1 \text{ mol } \text{Prod}} = 9.9 \text{ g } \text{Prod}
\]

Step 2) Theoretical Maximum and Limiting Reagent

Because 9.9 is smaller than 15, bromobenzene is the limiting reagent and the theoretical maximum amount of product which can form is 9.9 grams.

Step 3) Percent Yield. Using knowledge of actual amount of product formed, calculate the % yield.

\[
\frac{\text{Actual Mass Product Formed (g)}}{\text{Theoretical Maximum Mass Product (g)}} \times 100\% = \frac{6.655 \text{ g } \text{Product}}{9.9 \text{ g } \text{product}} \times 100\% = 67\% \text{ yield}
\]

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