Theoretical Yield: Example 3

If you begin with 25 mL of propionic acid, 20 mL of n-butanol, 1 ml of sulfuric acid, what is the theoretical yield of n-butylpropionate in the following acid-catalyzed esterification?

\[ \text{H}_2\text{CCH}_2\text{COOH} + \text{CH}_3\text{CH}_2\text{CH}_2\text{OH} \xrightarrow{\text{H}^+} \text{CH}_3\text{CH}_2\text{C}-(\text{CH}_2)\text{CH}_2 \text{OH} \]

The reaction as written above is balanced, with one mole of propionic acid and one mole of n-butanol producing one mole of n-butylpropionate and one mole of water, therefore the stoichiometry is 1:1. The mineral acid (sulfuric acid), written over the arrow, is a catalyst and does not enter into the theoretical yield calculations. Next, determine the number of moles of each reactant. To do this, consult the Tables of Physical Constants:

<table>
<thead>
<tr>
<th>compound</th>
<th>MW</th>
<th>density</th>
</tr>
</thead>
<tbody>
<tr>
<td>propionic acid</td>
<td>74.08</td>
<td>0.993</td>
</tr>
<tr>
<td>n-butanol</td>
<td>74.12</td>
<td>0.8098</td>
</tr>
<tr>
<td>n-butylpropionate</td>
<td>130.19</td>
<td>0.875</td>
</tr>
</tbody>
</table>

25 mL of propionic acid is will produce 0.335 mole of n-butylpropionate:

\[
25 \text{ mL} \times \frac{0.993 \text{ g}}{\text{mL}} \times \frac{\text{mole}}{74.08 \text{ g}} = 0.335 \text{ mole}
\]

20 mL of n-butanol will produce 0.218 mole of n-butylpropionate:

\[
20 \text{ mL} \times \frac{0.8094 \text{ g}}{\text{mL}} \times \frac{\text{mole}}{74.12 \text{ g}} = 0.218 \text{ mole}
\]

Therefore, the n-butanol is the limiting reagent: only 0.218 mole of n-butylpropionate can be produced using 0.218 moles of n-butanol and 0.335 moles of propionic acid. The theoretical yield is 28.4 gram:

\[
0.218 \text{ mole} \times \frac{130 \text{ g}}{1 \text{ mole}} = 28.4 \text{ g}
\]

From: [http://orgchem.colorado.edu/hndbksupport/labnb/tyex3.html](http://orgchem.colorado.edu/hndbksupport/labnb/tyex3.html)