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Understanding the concept of yield in chemistry is fundamental for both students and professionals working in chemical synthesis and manufacturing. Theoretical yield, in particular, represents the maximum amount of product that can be obtained from a given amount of reactants, assuming perfect conditions with no losses. When performing a synthesis such as the production of acetylsalicylic acid, commonly known as aspirin, calculating the percent yield provides insight into the efficiency of the reaction process.

In this article, we will walk through the process of calculating the percent yield of acetylsalicylic acid when the theoretical yield is known. We will explore the relevant chemical formulas, stoichiometry calculations, and practical considerations to deepen your understanding of this essential concept in organic synthesis.

Understanding the Basics of Yield in Chemical Reactions

What Is Theoretical Yield?

Theoretical yield is the maximum amount of product that could be formed in a chemical reaction based on the stoichiometry of the balanced chemical equation. It is calculated assuming that the limiting reactant is completely consumed and no side reactions or losses occur.

What Is Actual Yield?

Actual yield is the measured amount of product obtained from a real experiment. Due to practical factors such as impurities, incomplete reactions, and procedural losses, the actual yield is often less than the theoretical yield.

What Is Percent Yield?

Percent yield quantifies the efficiency of a reaction:

$$\text{Percent Yield} = \left(\frac{\text{Actual Yield}}{\text{Theoretical Yield}} \right) \times 100\%$$

Knowing the percent yield helps chemists evaluate and optimize synthesis procedures.

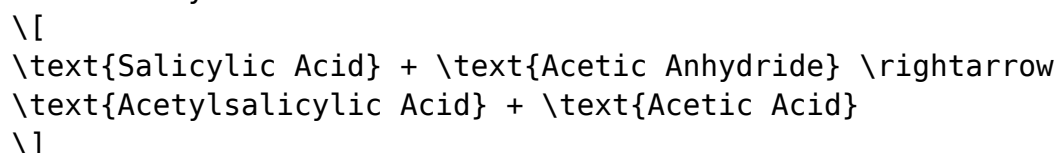
Calculating Theoretical Yield of Acetylsalicylic Acid

Suppose you are given that the theoretical yield of acetylsalicylic acid (aspirin) is 2.417 grams. To find the percent yield, you need the actual yield from the experiment. However, in some problems, only the theoretical yield and other data are provided, and the goal is to understand the calculation process.

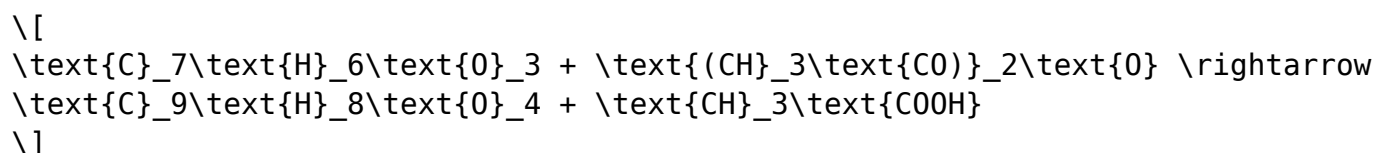
Let's walk through how to determine the percent yield based on given or assumed actual yields.

Step 1: Write the Balanced Chemical Equation

The synthesis of acetylsalicylic acid involves reacting salicylic acid with acetic anhydride:



The balanced reaction:



This indicates a 1:1 molar ratio between salicylic acid and acetylsalicylic acid.

Step 2: Determine Molar Masses

- Acetylsalicylic acid (aspirin), $\text{C}_9\text{H}_8\text{O}_4$:

$$(9 \times 12.01) + (8 \times 1.008) + (4 \times 16.00) = 108.09 + 8.064 + 64.00 = 180.154 \text{ g/mol}$$

- Salicylic acid, $C_7H_6O_3$:

$$(7 \times 12.01) + (6 \times 1.008) + (3 \times 16.00) = 84.07 + 6.048 + 48.00 = 138.118 \text{ g/mol}$$

\]

- Acetic anhydride, $(CH_3CO)_2O$:

$$(2 \times (12.01 + 3 \times 1.008 + 16.00)) + 16.00 = (2 \times (12.01 + 3.024 + 16.00)) + 16.00$$

\]

\[

$$(2 \times 31.034) + 16.00 = 62.068 + 16.00 = 78.068 \text{ g/mol}$$

\]

Step 3: Use Moles to Relate Reactants and Products

Since the molar ratio between salicylic acid and aspirin is 1:1, the amount of aspirin produced theoretically depends on the amount of salicylic acid used.

Suppose the starting amount of salicylic acid is known; then:

\[

$$\text{Moles of salicylic acid} = \frac{\text{Mass of salicylic acid}}{\text{Molar mass of salicylic acid}}$$

\]

The number of moles of aspirin (theoretical yield) is equal to the moles of salicylic acid reacted, assuming complete reaction.

Finally, the theoretical mass of aspirin:

\[

$$\text{Mass of aspirin} = \text{Moles of aspirin} \times \text{Molar mass of aspirin}$$

\]

Given the theoretical yield of 2.417 grams, we can work backwards to find the amount of reactants used if needed.

Calculating Percent Yield

To finalize the calculation, you need the actual yield. For example, assume the actual yield obtained from the experiment is 2.0 grams.

Using the formula:

\[

$$\text{Percent Yield} = \left(\frac{\text{Actual Yield}}{\text{Theoretical Yield}} \right) \times 100\%$$

\]

Plugging in the values:

\[
\text{Percent Yield} = \left(\frac{2.0\text{g}}{2.417\text{g}} \right) \times 100\% \approx 82.77\%
\]

Thus, the percent yield of acetylsalicylic acid in this case would be approximately 82.77%.

Factors Affecting the Percent Yield in Aspirin Synthesis

Achieving a high percent yield depends on several factors:

- Purity of reactants: Impurities can reduce yield.
- Reaction conditions: Temperature, time, and solvent choice influence the reaction completeness.
- Reaction completion: Ensuring the reaction goes to completion minimizes unreacted starting material.
- Isolation and purification: Losses during filtration, washing, or recrystallization reduce actual yield.
- Side reactions: Unwanted reactions can produce by-products, decreasing the yield.

Practical Tips for Maximizing Yield in Aspirin Synthesis

- Use high-purity reagents.
- Maintain optimal reaction temperatures.
- Use precise measurements for reactants.
- Allow sufficient reaction time.
- Carefully isolate and purify the product to minimize losses.
- Recrystallize the product to improve purity and yield.

Summary and Final Thoughts

Calculating the percent yield of acetylsalicylic acid from a known theoretical yield involves understanding the stoichiometry of the reaction, accurately measuring actual product obtained, and applying the formula:

\[
\text{Percent Yield} = \left(\frac{\text{Actual Yield}}{\text{Theoretical Yield}} \right) \times 100\%
\]

\]

In our example, assuming an actual yield of 2.0 grams with a theoretical yield of 2.417 grams, the percent yield is approximately 82.77%. This indicates a relatively efficient synthesis process, with room for optimization to improve the yield further.

Understanding and calculating percent yield not only helps chemists evaluate their experimental success but also guides improvements in synthesis techniques, contributing to more sustainable and cost-effective chemical manufacturing.

Keywords: percent yield, theoretical yield, acetylsalicylic acid, aspirin, chemical synthesis, stoichiometry, organic chemistry, reaction efficiency, yield calculation

Frequently Asked Questions

What is the theoretical yield of acetylsalicylic acid given as 2.417 g?

The theoretical yield provided is 2.417 grams of acetylsalicylic acid.

How do you calculate the percent yield of acetylsalicylic acid?

Percent yield is calculated by dividing the actual yield by the theoretical yield and multiplying by 100: $(\text{Actual Yield} / \text{Theoretical Yield}) \times 100\%$.

If the actual yield of acetylsalicylic acid obtained is 2.0 g, what is the percent yield?

Percent yield = $(2.0 \text{ g} / 2.417 \text{ g}) \times 100\% \approx 82.75\%$.

Why is it important to calculate the percent yield in a chemical synthesis?

Calculating percent yield helps evaluate the efficiency of the reaction and identify losses or side reactions during the process.

What factors can affect the percent yield of

acetylsalicylic acid in synthesis?

Factors include incomplete reactions, side reactions, impurities, measurement errors, and losses during transfer or purification.

Can the theoretical yield of 2.417 g of acetylsalicylic acid be achieved in practice?

Usually, the theoretical yield is an ideal maximum; actual yields are often lower due to practical limitations, so achieving 100% is unlikely.

How do you determine the actual yield needed to find the percent yield if the theoretical yield is 2.417 g?

You need to know the actual amount of acetylsalicylic acid obtained from the reaction; then, use the formula: $(\text{Actual Yield} / 2.417 \text{ g}) \times 100\%$.

What steps can be taken to improve the percent yield of acetylsalicylic acid synthesis?

Optimizing reaction conditions, ensuring complete reactions, minimizing losses during purification, and using pure reagents can improve yield.

Additional Resources

Understanding the Percent Yield Calculation of Acetylsalicylic Acid: A Comprehensive Guide

When delving into the world of chemistry, especially in the realm of organic synthesis, understanding the concept of yield—particularly percent yield—is fundamental. The synthesis of acetylsalicylic acid (commonly known as aspirin) provides a classic example of applying theoretical calculations to real-world laboratory results. In this detailed exploration, we will analyze how to determine the percent yield of acetylsalicylic acid given a theoretical yield of 2.417 grams, breaking down the process step-by-step, and elaborating on the critical concepts involved.

Introduction to Yield in Chemical Reactions

Before diving into calculations, it's essential to clarify what is meant by theoretical yield and percent yield in chemistry:

- Theoretical Yield: The maximum amount of product that can be formed from a given amount of reactants, based on the stoichiometry of the balanced chemical equation. It assumes perfect conditions with no losses or side reactions.

- Actual Yield: The amount of product actually obtained from the reaction under practical, real-world conditions.

- Percent Yield: A measure of the efficiency of a reaction, calculated as:

$$\text{Percent Yield} = \left(\frac{\text{Actual Yield}}{\text{Theoretical Yield}} \right) \times 100\%$$

In this context, the theoretical yield of acetylsalicylic acid has been given as 2.417 grams, and our goal is to determine the percent yield based on the actual yield obtained experimentally.

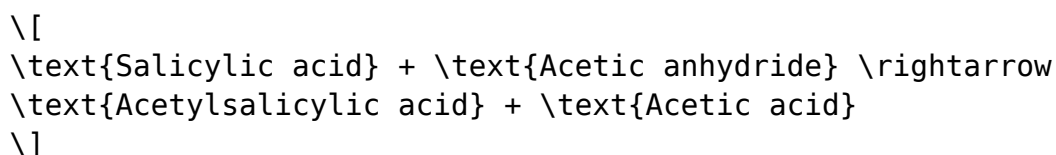
Background on Acetylsalicylic Acid Synthesis

Understanding the synthesis pathway helps in grasping the stoichiometry involved:

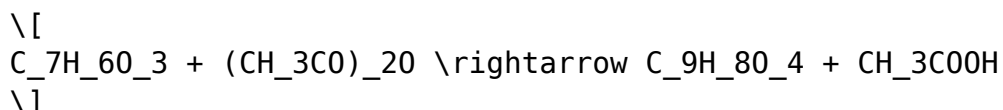
1. Starting Materials:

- Salicylic acid ($\text{C}_7\text{H}_6\text{O}_3$)
- Acetic anhydride ($\text{C}_4\text{H}_6\text{O}_3$)

2. Reaction Overview:



3. Balanced Chemical Equation:



This reaction typically proceeds with a molar ratio of 1:1:1:1, meaning one mole of salicylic acid reacts with one mole of acetic anhydride to produce one mole of acetylsalicylic acid and one mole of acetic acid.

Calculating Theoretical Yield of Acetylsalicylic Acid

Step 1: Identify the Molar Masses

- Salicylic acid ($C_7H_6O_3$):

$$\begin{aligned} & (7 \times 12.01) + (6 \times 1.008) + (3 \times 16.00) = 84.07 + 6.048 + \\ & 48.00 = 138.118 \text{ g/mol} \end{aligned}$$

- Acetylsalicylic acid ($C_9H_8O_4$):

$$\begin{aligned} & (9 \times 12.01) + (8 \times 1.008) + (4 \times 16.00) = 108.09 + 8.064 + \\ & 64.00 = 180.154 \text{ g/mol} \end{aligned}$$

- Acetic anhydride ($C_4H_6O_3$):

$$\begin{aligned} & (4 \times 12.01) + (6 \times 1.008) + (3 \times 16.00) = 48.04 + 6.048 + \\ & 48.00 = 102.088 \text{ g/mol} \end{aligned}$$

Step 2: Determine the Limiting Reactant

Suppose you start with a known amount of salicylic acid. For simplicity, assume the initial amount of salicylic acid is the limiting reagent, or that the reaction has proceeded with a known amount of salicylic acid.

Step 3: Calculate Moles of Salicylic Acid

If the starting amount of salicylic acid is known, say, x grams, then:

$$\text{Moles of salicylic acid} = \frac{x}{138.118}$$

Step 4: Theoretical Yield Calculation

Since the molar ratio is 1:1 between salicylic acid and acetylsalicylic acid:

$$\text{Moles of acetylsalicylic acid} = \text{Moles of salicylic acid}$$

Thus, the theoretical mass of acetylsalicylic acid:

$$\text{Theoretical yield} = \text{Moles of acetylsalicylic acid} \times 180.154$$

Given that the theoretical yield has been calculated or provided as 2.417 grams, this indicates that the initial amount of salicylic acid used corresponds to:

$$\text{Moles of salicylic acid} = \frac{2.417}{180.154} \approx 0.0134 \text{ mol}$$

Correspondingly, the initial mass of salicylic acid used was:

$$138.118 \times 0.0134 \approx 1.85 \text{ g}$$

Calculating Percent Yield

With the theoretical yield established at 2.417 g, the next step involves incorporating the actual yield obtained from experimental procedures.

Step 1: Obtain Actual Yield

Assuming an experimental process yields, for example, 1.8 grams of acetylsalicylic acid.

Step 2: Apply the Percent Yield Formula

$$\text{Percent Yield} = \left(\frac{\text{Actual Yield}}{\text{Theoretical Yield}} \right) \times 100\%$$

$$\text{Percent Yield} = \left(\frac{1.8}{2.417} \right) \times 100\% \approx 74.45\%$$

This indicates that approximately 74.45% of the theoretical maximum amount of acetylsalicylic acid was obtained in the experiment.

Factors Influencing Yield in Aspirin Synthesis

The percentage yield can vary significantly based on numerous factors, including:

- Purity of Reactants: Impurities can lead to side reactions or incomplete reactions.
- Reaction Conditions: Temperature, solvent, and reaction time can influence the efficiency.
- Reaction Technique: Stirring, addition rate, and mixing impact conversion rates.
- Work-up and Purification: Losses during filtration, washing, and recrystallization reduce the actual yield.
- Side Reactions: Formation of by-products or degradation of the product.

Understanding these factors helps optimize conditions to maximize yield.

Real-World Applications and Significance of Percent Yield

Calculating and understanding percent yield is critical in both academic and industrial settings:

- Academic Laboratory: Helps students understand reaction efficiency and troubleshoot synthesis procedures.
- Pharmaceutical Industry: Ensures cost-effective production and adherence to quality standards.
- Research and Development: Guides modifications to improve synthetic pathways.

An accurate percent yield also informs economic feasibility and process optimization.

Advanced Considerations

For more precise calculations, consider:

- Molecular Purity: Actual yield should be corrected for purity via techniques like melting point analysis or spectroscopic methods.
- Yield Losses: Quantify losses during each step to identify bottlenecks.
- Theoretical vs. Actual: Discrepancies highlight process inefficiencies or

procedural errors.

In complex syntheses, the calculation becomes more nuanced, involving multiple steps and reagents.

Conclusion

In summary, determining the percent yield of acetylsalicylic acid when the theoretical yield is known involves a fundamental understanding of stoichiometry, careful calculation, and consideration of practical factors affecting the reaction. Given a theoretical yield of 2.417 grams, if the actual yield obtained from the experiment is, for example, 1.8 grams, the percent yield would be approximately 74.45%. This value provides insight into the efficiency of the synthesis process and guides improvements for future experiments.

Mastering these calculations not only enhances one's grasp of organic chemistry principles but also equips chemists with the tools necessary for process optimization, quality control, and cost management in pharmaceutical manufacturing and research. The ability to analyze and interpret percent yield data ultimately advances both academic understanding and industrial application of chemical syntheses such as that of acetylsalicylic acid.

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