Using The Following Reaction, Determine The Theoretical Yield Of Acetylsalicylic Acid If Given 2.31 Grams

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Understanding how to determine the theoretical yield of a chemical compound is fundamental in chemistry, especially in reactions involving organic synthesis such as the production of acetylsalicylic acid, commonly known as aspirin. When given a specific amount of reactant—in this case, 2.31 grams—it is essential to analyze the chemical reaction, calculate molar quantities, and apply stoichiometry principles to predict the maximum amount of product that can be formed under ideal conditions. This comprehensive guide will walk you through the process of calculating the theoretical yield of acetylsalicylic acid based on a given mass of starting material, emphasizing the importance of each step and providing tips for accurate computation.

Understanding the Reaction: Synthesis of Acetylsalicylic Acid

Before diving into calculations, it is crucial to understand the chemical reaction involved in synthesizing acetylsalicylic acid. The process typically involves the acetylation of salicylic acid with acetic anhydride, catalyzed by sulfuric acid or phosphoric acid.

The Chemical Equation

The balanced chemical equation for the synthesis is:

$$\text{Salicylic Acid } (C}_7\text{H}_6\text{O}_3) + \text{Acetic Anhydride } (C}_4\text{H}_6\text{O}_3) \rightarrow \text{Acetylsalicylic Acid } (C}_9\text{H}_8\text{O}_4) + \text{Acetic Acid } (C}_2\text{H}_4\text{O}_2)$$

This indicates that:

- 1 mole of salicylic acid reacts with 1 mole of acetic anhydride to produce 1 mole of acetylsalicylic acid and 1 mole of acetic acid.

Step-by-Step Calculation of Theoretical Yield

Calculating the theoretical yield involves several key steps:

1. Identify the limiting reactant (if multiple reactants are involved).
2. Determine the molar mass of the reactant and product.
3. Convert the given mass of reactant to moles.
4. Use stoichiometry to find moles of product formed.
5. Convert moles of product to grams to find the theoretical yield.

Since the problem provides 2.31 grams of salicylic acid, and assuming excess acetic anhydride, salicylic acid is the limiting reactant.

Calculating the Molar Masses

Accurate molar mass calculations are essential for precise results.

Molar Mass of Salicylic Acid ($C_7H_6O_3$)

- Carbon (C): 12.01 g/mol × 7 = 84.07 g/mol
- Hydrogen (H): 1.008 g/mol × 6 = 6.048 g/mol
- Oxygen (O): 16.00 g/mol × 3 = 48.00 g/mol

Total molar mass: 84.07 + 6.048 + 48.00 = 138.118 g/mol

Molar Mass of Acetylsalicylic Acid ($C_9H_8O_4$)

- Carbon (C): 12.01 g/mol × 9 = 108.09 g/mol
- Hydrogen (H): 1.008 g/mol × 8 = 8.064 g/mol
- Oxygen (O): 16.00 g/mol × 4 = 64.00 g/mol

Total molar mass: 108.09 + 8.064 + 64.00 = 180.154 g/mol

Calculating Moles of Salicylic Acid

Given mass of salicylic acid = 2.31 grams

Number of moles:

$$
\text{Moles of salicylic acid} = \frac{\text{Mass}}{\text{Molar mass}} = \frac{2.31\, \text{g}}{138.118\, \text{g/mol}} \approx 0.01673\, \text{mol}
$$

Applying Stoichiometry to Find Moles of Acetylsalicylic Acid

From the balanced chemical equation, the molar ratio of salicylic acid to acetylsalicylic acid is 1:1.

Therefore:

$$
\text{Moles of acetylsalicylic acid} = \text{Moles of salicylic acid} = 0.01673\, \text{mol}
$$

Calculating the Theoretical Yield in Grams

Using the molar mass of acetylsalicylic acid:

$$
\text{Mass} = \text{Moles} \times \text{Molar mass} = 0.01673\, \text{mol} \times 180.154\, \text{g/mol} \approx 3.015\, \text{g}
$$

Thus, the theoretical yield of acetylsalicylic acid is approximately 3.02 grams.

Additional Considerations for Accurate Yield Calculation

While the above calculations assume ideal conditions, real-world factors can influence actual yields. It's important to understand these considerations:

- **Purity of Reactants:** Impurities can reduce the actual yield.
- **Reaction Conditions:** Temperature, solvent, and catalyst can impact the reaction efficiency.
- **Side Reactions:** Competing reactions may produce byproducts, lowering the yield.
- **Measurement Accuracy:** Precise weighing and measurement are critical for accurate calculations.

Summary: How to Determine Theoretical Yield of Acetylsalicylic Acid

To summarize, the process involves:

1. Understanding the balanced chemical reaction involved in aspirin synthesis.
2. Calculating the molar mass of the limiting reactant (salicylic acid).
3. Converting the given mass of the reactant to moles.
4. Applying the molar ratio from the balanced equation to find moles of aspirin produced.
5. Converting moles of aspirin to grams using its molar mass to determine the theoretical yield.

Using this method, given 2.31 grams of salicylic acid, the maximum amount of acetylsalicylic acid that can theoretically be produced is approximately 3.02 grams under ideal conditions.

Practical Implications and Usage

Understanding how to calculate the theoretical yield is vital in laboratory and industrial settings for:

- Planning the amount of reactants needed for syntheses.
- Estimating potential product output.
- Evaluating the efficiency of the reaction by comparing actual yields to theoretical yields.
- Optimizing reaction conditions to maximize product recovery.

Conclusion

Determining the theoretical yield of acetylsalicylic acid from a given mass of salicylic acid involves a clear understanding of the chemical reaction, precise molar mass calculations, and stoichiometric relationships. By following the step-by-step process outlined in this guide, chemists and students can accurately predict the maximum amount of aspirin that can be produced, aiding in planning and analysis of chemical syntheses. Remember, the theoretical yield represents an ideal scenario; real yields will often be lower due to practical limitations, but knowing the maximum potential helps in evaluating reaction efficiency and optimizing processes.

Keywords: theoretical yield, acetylsalicylic acid, aspirin synthesis, stoichiometry, molar mass, chemical reaction, limiting reactant, organic chemistry, reaction yield calculation

Frequently Asked Questions

What is the balanced chemical equation for the synthesis of acetylsalicylic acid?

The balanced chemical equation is: Salicylic acid + Acetic anhydride → Acetylsalicylic acid + Acetic acid.

How do you calculate the molar mass of acetylsalicylic acid?

The molar mass of acetylsalicylic acid ($C_9H_8O_4$) is approximately 180.16 g/mol, calculated by summing the atomic masses: (9×12.01) + (8×1.008) + (4×16.00).

What is the theoretical yield and how is it determined in this reaction?

The theoretical yield is the maximum amount of acetylsalicylic acid that can be produced from a given amount of reactant, calculated by converting the given mass to moles and using stoichiometry based on the balanced equation.

How do you use the given 2.31 grams of salicylic acid to find the theoretical yield?

First, convert 2.31 grams of salicylic acid to moles: 2.31 g / 138.12 g/mol (molar mass of salicylic acid). Then, use the molar ratio from the balanced equation to find the moles of acetylsalicylic acid produced, and convert back to grams.

What assumptions are made when calculating the theoretical yield in this reaction?

It is assumed that the reaction goes to completion with 100% efficiency, no side reactions occur, and all reactants are pure and available in the specified amounts.

What is the final step to determine the theoretical yield in grams after calculating moles?

Multiply the moles of acetylsalicylic acid obtained by its molar mass (180.16 g/mol) to get the theoretical yield in grams.

Additional Resources

Using The Following Reaction, Determine The Theoretical Yield Of Acetylsalicylic Acid If Given 2.31 Grams

Understanding the theoretical yield of a chemical reaction is fundamental in the field of chemistry, especially in organic synthesis and pharmaceutical manufacturing. In this detailed exploration, we will analyze how to determine the theoretical yield of acetylsalicylic acid (aspirin) starting from a given mass of reactant, specifically 2.31 grams. This comprehensive review will cover the principles of stoichiometry, the specific chemical reaction involved, molar calculations, and considerations for practical applications.

Overview of Acetylsalicylic Acid and Its Significance

Acetylsalicylic acid, commonly known as aspirin, is a widely used analgesic, anti-inflammatory, and antipyretic agent. Its synthesis is a classic example used in organic chemistry laboratories to teach stoichiometry and reaction mechanisms.

- Historical context: Derived historically from willow bark extracts, aspirin was synthesized in the late 19th century.
- Medical importance: Its widespread use includes pain relief, reduction of inflammation, and prevention of blood clots.
- Chemical structure: It is an ester formed from salicylic acid and acetic anhydride.

Understanding the synthesis and yield calculations is essential for both academic purposes and industrial production, where maximizing efficiency and minimizing waste are key.

The Chemical Reaction Involved

The synthesis of acetylsalicylic acid primarily involves the acetylation of salicylic acid with acetic anhydride.

Reaction Equation:

$$\text{Salicylic acid} + \text{Acetic anhydride} \rightarrow \text{Acetylsalicylic acid} + \text{Acetic acid}$$

Expressed chemically:

$$\text{C}_7\text{H}_6\text{O}_3 + \text{(CH}_3\text{CO)}_2\text{O} \rightarrow \text{C}_9\text{H}_8\text{O}_4 + \text{CH}_3\text{COOH}$$

Key points:

- Reactants:
- Salicylic acid ($C_7H_6O_3$)
- Acetic anhydride ($(CH_3CO)_2O$)
- Products:
- Acetylsalicylic acid (aspirin, $C_9H_8O_4$)
- Acetic acid (CH_3COOH)

Note: For simplicity, this calculation assumes pure reactants and complete reaction without side reactions or losses.

Determining the Theoretical Yield: Step-by-Step Approach

Calculating the theoretical yield involves a systematic approach:

1. Identify the limiting reactant (if multiple reactants are involved).
2. Convert the given mass of reactant to moles.
3. Use stoichiometry from the balanced chemical equation to find moles of product formed.
4. Convert moles of product to grams to find the theoretical yield.

Since the problem emphasizes starting with 2.31 grams of a reactant, we need to clarify which reactant we are considering. For this review, let's assume that the 2.31 grams given is of salicylic acid, the limiting reactant, as it is often the initial reactant in aspirin synthesis.

Step 1: Write the Balanced Chemical Equation

The reaction is already balanced as:

$$\text{C}_7\text{H}_6\text{O}_3 + \text{(CH}_3\text{CO)}_2\text{O} \rightarrow \text{C}_9\text{H}_8\text{O}_4 + \text{CH}_3\text{COOH}$$

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

Step 2: Calculate Moles of Salicylic Acid (Reactant)

- Given mass of salicylic acid: 2.31 grams
- Molar mass of salicylic acid ($C_7H_6O_3$):

Calculations:
- Carbon (C): 7 atoms × 12.01 g/mol = 84.07 g/mol
- Hydrogen (H): 6 atoms × 1.008 g/mol = 6.048 g/mol

- Oxygen (O): 3 atoms × 16.00 g/mol = 48.00 g/mol

Total molar mass:
$$ 84.07 + 6.048 + 48.00 = 138.118\, \text{g/mol} $$

- Number of moles of salicylic acid:

$$
\text{Moles} = \frac{\text{Mass}}{\text{Molar mass}} = \frac{2.31\, \text{g}}{138.118\, \text{g/mol}} \approx 0.01673\, \text{mol}
$$

Step 3: Use Stoichiometry to Find Moles of Acetylsalicylic Acid

Since the molar ratio of salicylic acid to aspirin is 1:1:

$$
\text{Moles of aspirin} = \text{Moles of salicylic acid} = 0.01673\, \text{mol}
$$

Step 4: Convert Moles of Aspirin to Grams for Theoretical Yield

- Molar mass of acetylsalicylic acid ($C_9H_8O_4$):

Calculations:
- Carbon (C): 9 × 12.01 = 108.09 g/mol
- Hydrogen (H): 8 × 1.008 = 8.064 g/mol
- Oxygen (O): 4 × 16.00 = 64.00 g/mol

Total molar mass:
$$ 108.09 + 8.064 + 64.00 = 180.154\, \text{g/mol} $$

- Mass of aspirin (theoretical yield):

$$
\text{Mass} = \text{Moles} \times \text{Molar mass} = 0.01673\, \text{mol} \times 180.154\, \text{g/mol} \approx 3.013\, \text{g}
$$

Summary of the Calculation

- Initial amount of salicylic acid: 2.31 grams
- Moles of salicylic acid: approximately 0.01673 mol
- Moles of aspirin expected (theoretical maximum): 0.01673 mol
- Theoretical yield of aspirin: approximately 3.013 grams

This means, if the reaction proceeds perfectly with 100% efficiency, the maximum amount of acetylsalicylic

acid that can be produced from 2.31 grams of salicylic acid is about 3.01 grams.

Factors Affecting Real-world Yield

While the theoretical yield provides an ideal maximum, real-world reactions often produce less due to various factors:

- Incomplete reactions: Not all reactants convert to products.
- Side reactions: Formation of by-products reduces yield.
- Loss during purification: Filtration, washing, and recrystallization can reduce recovery.
- Impurities: Contaminants can affect yield calculations and product purity.

Therefore, actual yields are typically lower than the theoretical yield, often expressed as a percentage called the percent yield.

Additional Considerations for Accurate Calculations

1. Purity of Reactants:

- If salicylic acid is not pure, adjustments must be made based on its purity percentage.

2. Excess Reagents:

- Acetic anhydride is often used in excess to push the reaction toward completion.

3. Reaction Conditions:

- Temperature, catalyst presence, and reaction time influence the yield.

4. Purification Techniques:

- Recrystallization and filtration efficiencies impact the actual recovered amount of aspirin.

Practical Applications of Theoretical Yield Calculations

Understanding and calculating the theoretical yield is crucial in:

- Industrial manufacturing: Ensuring efficient production and cost estimation.
- Laboratory synthesis: Planning experiments and estimating product quantities.
- Academic assessments: Demonstrating understanding of stoichiometry principles.
- Quality control: Comparing actual yields with theoretical values to assess reaction efficiency.

Conclusion

In summary, when starting with 2.31 grams of salicylic acid, the maximum theoretical yield of acetylsalicylic acid, assuming complete reaction and no losses, is approximately 3.01 grams. This calculation relies on fundamental stoichiometric principles, molar mass determination, and balanced chemical equations. While achieving this maximum in practice may be challenging, understanding the theoretical yield provides a benchmark against which actual yields can be compared, guiding improvements in reaction efficiency and purity.

This detailed process exemplifies the importance of stoichiometry in organic synthesis and highlights how fundamental chemical principles translate into practical outcomes in laboratory and industrial settings. Mastery of these calculations enables chemists to optimize reactions, estimate production costs,

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