A Grignard Synthesis Begins With 6.00 G Of Bromobenzene And Ends With 3.94 G Benzoic Acid. What Is The

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Understanding the transformation of organic compounds through Grignard reactions is fundamental in organic chemistry. This process not only exemplifies the versatility of Grignard reagents but also highlights key concepts such as stoichiometry, reaction mechanisms, and product analysis. In this comprehensive article, we will explore the detailed pathway starting with 6.00 grams of bromobenzene and culminating in the formation of 3.94 grams of benzoic acid. Our goal is to elucidate the underlying chemistry, calculations, and reasoning that lead to understanding the overall reaction process, yield, and the identity of the reagents involved.

Introduction to Grignard Reactions and Their Significance

Grignard reactions are a cornerstone of organic synthesis, allowing chemists to form carbon-carbon bonds by reacting organomagnesium halides—known as Grignard reagents—with various electrophiles. These reactions are highly valuable because they enable the formation of complex molecules from simple starting materials.

Developed by Victor Grignard in the early 20th century, Grignard reagents typically have the formula R–MgX, where R is an organic group and X is a halogen (Cl, Br, or I). They are highly reactive and require careful handling, usually under anhydrous conditions, due to their sensitivity to moisture.

The pathway from bromobenzene to benzoic acid involves multiple steps, often including the formation of a Grignard reagent, subsequent reactions with oxidizing agents or carbonyl compounds, and eventual oxidation to benzoic acid. Understanding this sequence is crucial for mastering organic synthesis techniques.

Step 1: Formation of the Grignard Reagent from Bromobenzene

The first step in the synthesis involves converting bromobenzene into phenylmagnesium bromide, a common Grignard reagent.

Reaction Conditions for Grignard Formation

- Reagents Needed:
- Bromobenzene (C_6H_5Br)
- Magnesium turnings (Mg)
- Anhydrous ether as solvent

- Reaction Process:
- Bromobenzene is added to magnesium turnings under an inert atmosphere (nitrogen or argon).
- The mixture is gently heated or stirred to initiate the formation of phenylmagnesium bromide.

Calculating the Moles of Bromobenzene

Given mass of bromobenzene = 6.00 g

- Molecular weight of bromobenzene (C_6H_5Br) = (6 × 12.01) + (5 × 1.008) + (79.904) ≈ 157.01 g/mol

Number of moles:

$$
\text{moles of bromobenzene} = \frac{6.00\, \text{g}}{157.01\, \text{g/mol}} \approx 0.0382\, \text{mol}
$$

Assuming complete conversion, the moles of phenylmagnesium bromide formed are also approximately 0.0382 mol.

Step 2: From Grignard Reagent to Benzoic Acid

The key conversion to benzoic acid involves oxidation of the phenylmagnesium bromide. Typically, Grignard reagents react with oxygen, carbon dioxide, or other oxidants to produce carboxylic acids.

Reaction Pathway

- The phenylmagnesium bromide reacts with an oxidizing agent (most commonly carbon dioxide, CO_2).
- After quenching the reaction with water or acid, benzoic acid is formed.

The overall reaction with CO_2:

$$
\text{C}_6\text{H}_5\text{MgBr} + \text{CO}_2 \rightarrow \text{C}_6\text{H}_5\text{COOH} + \text{MgBrOH}
$$

This process is known as carboxylation.

Calculating Theoretical Yield of Benzoic Acid

- Moles of phenylmagnesium bromide = 0.0382 mol
- Since the molar ratio of phenylmagnesium bromide to benzoic acid is 1:1, the theoretical moles of benzoic acid formed are also 0.0382 mol.

Molecular weight of benzoic acid (C_6H_5COOH):

$$
(6 \times 12.01) + (5 \times 1.008) + (12.01) + (16.00) \approx 122.12\, \text{g/mol}
$$

Theoretical mass:

$$
0.0382\, \text{mol} \times 122.12\, \text{g/mol} \approx 4.67\, \text{g}
$$

Step 3: Actual Yield and Yield Calculation

The actual yield of benzoic acid obtained is 3.94 g.

- Percentage yield:

$$
\text{Yield} = \frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100 = \frac{3.94}{4.67} \times 100 \approx 84.4\%
$$

This indicates an efficient synthesis with minimal losses.

Understanding the Reaction Mechanism and Key Concepts

1. Formation of the Grignard Reagent

- Bromobenzene reacts with magnesium in anhydrous ether.
- The reaction is initiated by small amounts of iodine or other activators to facilitate magnesium insertion.
- The phenylmagnesium bromide formed is a highly reactive nucleophile.

2. Carboxylation with CO_2

- The phenylmagnesium bromide attacks the electrophilic carbon in CO_2.
- This results in the formation of a magnesium phenolate intermediate.
- Acid work-up (adding dilute acid) converts the intermediate into benzoic acid.

3. Oxidation and Purification

- The crude product is purified via recrystallization.
- The purity affects the actual yield and quality.

Additional Considerations and Safety Precautions

- Grignard reagents are highly reactive with moisture; hence, reactions are performed under inert atmosphere.
- Handling magnesium turnings and ether requires caution due to flammability and toxicity.
- Proper disposal of reaction waste, especially magnesium salts, is essential.

Conclusion: What Is the Overall Reaction and Its Significance?

The transformation from bromobenzene to benzoic acid via Grignard chemistry exemplifies the power of organometallic reagents in organic synthesis. Starting with 6.00 grams of bromobenzene, the process yields approximately 3.94 grams of benzoic acid, reflecting an efficient reaction with an approximate yield of 84.4%.

This synthesis highlights several key principles:

- The importance of molar calculations in predicting product yields.
- The role of Grignard reagents as nucleophiles and their reactivity with electrophiles like CO_2.
- The necessity of controlling reaction conditions to maximize yield and purity.

Understanding this pathway not only deepens the comprehension of Grignard reactions but also demonstrates their practical application in synthesizing valuable organic acids such as benzoic acid, which has widespread uses in food preservation, pharmaceuticals, and chemical manufacturing.

In summary, starting with 6.00 g of bromobenzene, a typical Grignard synthesis involving formation of phenylmagnesium bromide, followed by carboxylation with CO_2, results in approximately 3.94 g of benzoic acid, illustrating a classic and instructive example of organic synthesis in action.

Keywords: Grignard reaction, bromobenzene, benzoic acid synthesis, organic chemistry,

stoichiometry, carboxylation, organometallic reagents, chemical yield, reaction mechanism

Frequently Asked Questions

What is the main purpose of the Grignard synthesis starting with bromobenzene and ending with benzoic acid?

The purpose is to convert bromobenzene into benzoic acid through a series of reactions involving Grignard reagents and oxidation steps.

How is bromobenzene converted into benzoic acid in a Grignard synthesis?

Bromobenzene is first reacted with magnesium to form phenylmagnesium bromide (a Grignard reagent), which then reacts with carbon dioxide (CO_2) to produce benzoic acid upon acid workup.

What is the significance of the initial 6.00 g of bromobenzene in the synthesis?

It represents the starting amount of bromobenzene used to generate the Grignard reagent for the synthesis process.

How do you determine the yield of benzoic acid from the given starting material?

By calculating the theoretical maximum amount of benzoic acid that can be formed from 6.00 g of bromobenzene, then comparing it to the actual 3.94 g obtained to find the percentage yield.

What is the molar mass of bromobenzene and benzoic acid, and why are they important?

Bromobenzene has a molar mass of approximately 157.01 g/mol, and benzoic acid about 122.12 g/mol. These are important for converting grams to moles to perform stoichiometric calculations.

What is the theoretical yield of benzoic acid from 6.00 g of bromobenzene?

Calculating based on molar ratios, the theoretical yield is approximately 4.66 g of benzoic acid, assuming 100% efficiency.

What does the difference between the theoretical and actual yield indicate?

It indicates the efficiency of the reaction process, with the actual yield (3.94 g) being less than the theoretical yield (approx. 4.66 g) due to losses or side reactions.

How is the Grignard reagent prepared in this synthesis?

By reacting bromobenzene with magnesium metal in an anhydrous solvent like diethyl ether, forming phenylmagnesium bromide.

What role does oxidation play in converting the Grignard intermediate to benzoic acid?

Oxidation, typically with CO_2 followed by acid workup, transforms the phenylmagnesium bromide into benzoic acid.

Why is it important to know the final mass of benzoic acid obtained in this synthesis?

It helps determine the reaction's yield and efficiency, and verifies the success of the synthesis process based on theoretical calculations.

Additional Resources

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Introduction

In the realm of organic synthesis, Grignard reactions hold a pivotal role due to their versatility in forming carbon-carbon bonds, enabling chemists to construct complex molecules from simpler precursors. The process begins with the preparation of a Grignard reagent—an organomagnesium halide—derived from an alkyl or aryl halide, such as bromobenzene. The reaction pathway often involves subsequent transformations, culminating in the formation of various functionalized organic compounds.

This article delves into a specific case study where a Grignard synthesis initiates with 6.00 grams of bromobenzene and concludes with 3.94 grams of benzoic acid. Through detailed analysis, we aim to elucidate the underlying reaction mechanisms, identify the chemical transformations involved, and compute the yield or efficiency of the synthesis. The comprehensive examination combines theoretical chemistry principles with practical insights, making it a valuable resource for students, educators, and practitioners alike.

Overview of the Reaction Sequence

The Starting Material: Bromobenzene

Bromobenzene (C_6H_5Br) is an aromatic halide, characterized by a bromine atom attached to a benzene ring. Its significance lies in its ability to act as a precursor to arylmagnesium bromide (Grignard reagent) upon reaction with magnesium metal.

Formation of the Grignard Reagent

The initial step involves reacting bromobenzene with magnesium turnings in an anhydrous ether solvent, typically diethyl ether or tetrahydrofuran (THF). This process generates phenylmagnesium bromide, an organomagnesium compound:

$$ \text{C}_6\text{H}_5\text{Br} + \text{Mg} \rightarrow \text{C}_6\text{H}_5\text{MgBr} $$

This reagent is highly nucleophilic and reactive, capable of attacking electrophilic centers in various molecules.

Subsequent Carboxylation and Oxidation

The key transformations leading to benzoic acid usually involve carboxylation of the phenylmagnesium bromide with carbon dioxide (CO_2), followed by acidification:

1. Carboxylation:

$$ \text{C}_6\text{H}_5\text{MgBr} + \text{CO}_2 \rightarrow \text{C}_6\text{H}_5\text{CO}_2\text{MgBr} $$

2. Acidification:

$$ \text{C}_6\text{H}_5\text{CO}_2\text{MgBr} + \text{H}_3\text{O}^+ \rightarrow \text{C}_6\text{H}_5\text{COOH} + \text{MgBrOH} $$

The net result is the conversion of bromobenzene into benzoic acid via magnesium-mediated carboxylation and acid hydrolysis.

Final Product: Benzoic Acid

Benzoic acid (C_6H_5COOH) is a aromatic carboxylic acid, widely used as a preservative and in organic synthesis. Its synthesis from bromobenzene via Grignard chemistry underscores the utility of organometallic reagents in aromatic substitution and functional group transformations.

Quantitative Analysis: From Starting Material to Final Product

Initial Quantities: Calculating Moles of Bromobenzene

Given data:

- Mass of bromobenzene = 6.00 g

Molecular weight of bromobenzene (C_6H_5Br):

$$ \text{C}_6\text{H}_5\text{Br} \rightarrow (6 \times 12.01) + (5 \times 1.008) + 79.904 = 186.03\, \text{g/mol} $$

Number of moles:

$$ \text{Moles of bromobenzene} = \frac{6.00\, \text{g}}{186.03\, \text{g/mol}} \approx 0.0323\, \text{mol} $$

Final Quantities: Calculating Moles of Benzoic Acid

Given final mass:

- Mass of benzoic acid = 3.94 g

Molecular weight of benzoic acid (C_6H_5COOH):

$$ (6 \times 12.01) + (5 \times 1.008) + (12.01) + (2 \times 16.00) = 122.12\, \text{g/mol} $$

Number of moles:

$$ \text{Moles of benzoic acid} = \frac{3.94\, \text{g}}{122.12\, \text{g/mol}} \approx 0.0323\, \text{mol} $$

Reaction Efficiency: Calculating the Overall Yield

The close match in moles (0.0323 mol of starting bromobenzene and 0.0323 mol of benzoic acid) suggests a near-quantitative conversion, assuming complete reaction and no significant side reactions or losses. The theoretical maximum yield corresponds to the moles of bromobenzene used, and the actual yield is based on the benzoic acid obtained.

Yield Calculation

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

Theoretical yield:

$$ \text{Theoretical mass of benzoic acid} = 0.0323\, \text{mol} \times 122.12\, \text{g/mol} \approx 3.94\, \text{g} $$

Actual yield:

$$ 3.94\, \text{g} $$

Therefore:

\[

$$\text{Percent yield} \approx \frac{3.94}{3.94} \times 100 = 100\%$$

This indicates a highly efficient synthesis, assuming ideal conditions.

Chemical Mechanisms and Pathways

Step 1: Formation of Phenylmagnesium Bromide

The initial step involves the reaction:

$$\text{C}_6\text{H}_5\text{Br} + \text{Mg} \rightarrow \text{C}_6\text{H}_5\text{MgBr}$$

This process is typically facilitated by gentle heating or activation of magnesium, often with iodine or a small amount of iodine to initiate the reaction.

Step 2: Carboxylation with Carbon Dioxide

The phenylmagnesium bromide acts as a nucleophile, attacking the electrophilic carbon in CO_2:

$$\text{C}_6\text{H}_5\text{MgBr} + \text{CO}_2 \rightarrow \text{C}_6\text{H}_5\text{CO}_2\text{MgBr}$$

This intermediate is a magnesium phenylcarboxylate, which upon hydrolysis yields benzoic acid.

Step 3: Acid Hydrolysis

Adding dilute acid (e.g., HCl or H_2SO_4) cleaves the magnesium salt, freeing benzoic acid:

$$\text{C}_6\text{H}_5\text{CO}_2\text{MgBr} + \text{H}_3\text{O}^+ \rightarrow \text{C}_6\text{H}_5\text{COOH} + \text{MgBrOH}$$

This step completes the synthesis, providing the final benzoic acid product.

Considerations and Potential Side Reactions

Side Reactions and Impurities

While the theoretical yield approximates 100%, practical considerations often limit the actual yield:

- Incomplete reaction: Not all bromobenzene may react, especially if magnesium activation is suboptimal.
- Side reactions: Over-oxidation or formation of biphenyl due to coupling reactions.
- Losses during workup: During extraction, filtration, and purification, some material may be lost.
- Impurities in starting materials: Contaminants could affect yield and purity.

Reaction Conditions

Optimizing parameters such as temperature, solvent purity, and reagent quality are critical for maximizing yield and purity.

Analytical Techniques for Confirmation

To verify the formation of benzoic acid and assess purity, chemists employ various analytical methods:

- Melting point determination: Pure benzoic acid melts at approximately 122°C.
- Spectroscopic analysis: Infrared (IR) spectroscopy confirms the presence of carboxylic acid functional groups.
- Nuclear Magnetic Resonance (NMR): Proton and carbon NMR provide structural confirmation.
- Thin Layer Chromatography (TLC): Assesses purity and reaction completeness.

Significance and Practical Applications

Educational Perspective

This synthesis exemplifies core principles in organic chemistry—organometallic reactions, carboxylation, and functional group transformations. It serves as an instructive model for students learning about synthetic pathways involving Grignard reagents.

Industrial Relevance

Benzoic acid is a key precursor in the manufacture of various derivatives, preservatives, and pharmaceuticals. Efficient synthesis routes, as illustrated, are vital for industrial

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