# Given That The Grignard Reaction Used 1.4555 G Phenyl Bromide, 10. G Carbon Dioxide, 0.5734 G Magnesium

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This article provides an in-depth analysis of a Grignard reaction involving phenyl bromide, magnesium, and carbon dioxide. It explores the stoichiometry of the reaction, the mechanisms involved, the calculations for theoretical yields, potential side reactions, and the practical considerations for executing this classic organic synthesis. Understanding these aspects is essential for chemists aiming to optimize reaction conditions, maximize yields, and comprehend the underlying chemistry of Grignard reagents.

## Overview of the Grignard Reaction

### What Is a Grignard Reagent?

The Grignard reagent is an organomagnesium halide, typically represented as R–MgX, where R is an organic group and X is a halogen (Cl, Br, or I). These reagents are pivotal in forming carbon-carbon bonds, enabling the synthesis of alcohols, carboxylic acids, and other functionalized molecules.

### General Mechanism of the Reaction with Carbon Dioxide

When a Grignard reagent reacts with carbon dioxide ($CO_2$), it undergoes nucleophilic attack on the electrophilic carbon of $CO_2$, leading to the formation of a magnesium carboxylate intermediate. Subsequent acid work-up yields a carboxylic acid.

The simplified overall reaction can be summarized as:

$$
\mathrm{R–MgX} + \mathrm{CO}_2 \rightarrow \mathrm{R–COO}^{-} \mathrm{MgX}^{+} \rightarrow \mathrm{R–COOH} \text{ (upon acidification)}
$$

# Given Data and Initial Calculations

## Masses of Reactants

- Phenyl bromide ($C_6H_5Br$): 1.4555 g
- Carbon dioxide ($CO_2$): 10.0 g
- Magnesium (Mg): 0.5734 g

## Molar Masses of Reactants

- Phenyl bromide ($C_6H_5Br$): approximately 157.01 g/mol
- Magnesium (Mg): 24.305 g/mol
- Carbon dioxide ($CO_2$): 44.01 g/mol

## Calculating Moles of Reactants

- Moles of phenyl bromide:
$$
\text{mol} = \frac{1.4555\, \text{g}}{157.01\, \text{g/mol}} \approx 0.00927\, \text{mol}
$$
- Moles of magnesium:
$$
\text{mol} = \frac{0.5734\, \text{g}}{24.305\, \text{g/mol}} \approx 0.02358\, \text{mol}
$$
- Moles of carbon dioxide:
$$
\text{mol} = \frac{10.0\, \text{g}}{44.01\, \text{g/mol}} \approx 0.2273\, \text{mol}
$$

# Stoichiometry of the Reaction

## Reaction Equation

The overall reaction involves phenyl bromide reacting with magnesium to form phenylmagnesium bromide (a Grignard reagent), which then reacts with $CO_2$:

1. Formation of phenylmagnesium bromide:
\[

\mathrm{C_6H_5Br} + \mathrm{Mg} \rightarrow \mathrm{C_6H_5MgBr}
\]
2. Reaction with $CO_2$:
\[
\mathrm{C_6H_5MgBr} + \mathrm{CO}_2 \rightarrow \mathrm{C_6H_5COO}^{-} \mathrm{MgBr}^{+}
\]
3. Acid work-up:
\[
\mathrm{C_6H_5COO}^{-} \mathrm{MgBr}^{+} + \mathrm{H^+} \rightarrow \mathrm{C_6H_5COOH} + \mathrm{MgBr(OH)} \text{ (or similar)}
\]

Note: The molar ratio indicates that 1 mol of phenyl bromide reacts with 1 mol of magnesium to produce 1 mol of phenylmagnesium bromide, which then reacts with 1 mol of $CO_2$.

## Limiting Reagent Analysis

- The key limiting reagent is phenyl bromide, with 0.00927 mol.
- Magnesium is in excess: 0.02358 mol available.
- Carbon dioxide is in large excess: 0.2273 mol available.

Thus, the maximum theoretical amount of phenylacetic acid (or phenyl carboxylic acid) formed is based on the phenyl bromide amount.

# Calculations of Theoretical Yield

## Theoretical Moles of Product

Since phenyl bromide is limiting:
\[
\text{Moles of phenylacetic acid} = 0.00927\, \text{mol}
\]

## Molar Mass of Phenylacetic Acid

- Phenylacetic acid ($C_8H_8O_2$): approximately 136.15 g/mol

## Mass of Product (Theoretical Yield)

$$
\text{Mass} = 0.00927\, \text{mol} \times 136.15\, \text{g/mol} \approx 1.262\, \text{g}
$$

Therefore, the maximum theoretical yield of phenylacetic acid is approximately 1.262 grams.

# Practical Considerations and Reaction Efficiency

## Factors Affecting Yield

- Purity of phenyl bromide
- Quality of magnesium turnings
- Reaction conditions (solvent, temperature, atmosphere)
- Complete formation of the Grignard reagent
- Excess $CO_2$ ensuring complete reaction
- Work-up and purification procedures

## Possible Side Reactions

- Wurtz-type coupling, leading to biphenyl formation
- Hydrolysis of the Grignard reagent if moisture is present
- Formation of magnesium salts or oxides
- Overreaction or polymerization under harsh conditions

# Reaction Mechanism in Detail

## Formation of the Grignard Reagent

The initiation involves magnesium metal surface reacting with phenyl bromide:

$$
\mathrm{C_6H_5Br} + \mathrm{Mg} \rightarrow \mathrm{C_6H_5MgBr}
$$

This step may require activation (e.g., iodine, iodine solution, or sonication).

## Reaction with Carbon Dioxide

Nucleophilic attack:

$$
\mathrm{C_6H_5MgBr} + \mathrm{CO}_2 \rightarrow \mathrm{C_6H_5-COO}^{-} \mathrm{MgBr}^{+}
$$

Followed by acid work-up:

$$
\mathrm{C_6H_5-COO}^{-} \mathrm{MgBr}^{+} + \mathrm{H^+} \rightarrow \mathrm{C_6H_5COOH} + \mathrm{MgBr(OH)} \text{ or similar}
$$

Note: The acid work-up typically involves dilute acid (e.g., HCl or $H_2SO_4$) to protonate the carboxylate and release the acid.

# Safety and Handling

## Precautions When Handling Reactants

- Phenyl bromide is toxic and should be handled in a well-ventilated fume hood.
- Magnesium powder is reactive and can ignite if dry and finely divided.
- Carbon dioxide is a gas that can displace oxygen; proper ventilation is necessary.
- Organometallic reagents are highly reactive toward moisture and air; use dry glassware and inert atmosphere.

## Waste Disposal

- Magnesium salts and residual organometallic compounds should be disposed of following laboratory safety protocols.
- Acidic waste should be neutralized before disposal.

# Conclusion

This detailed analysis underscores the importance of precise measurements, understanding reaction mechanisms, and accounting for stoichiometry in Grignard reactions. Starting with 1.4555 g phenyl bromide, the theoretical maximum yield of phenylacetic acid is approximately 1.262 g, assuming complete conversion and ideal conditions. The excess magnesium and $CO_2$ ensure that phenyl bromide is the limiting reagent, making it the key factor in determining the maximum possible product yield. By carefully controlling reaction parameters and minimizing side reactions, chemists can optimize the efficiency of this classic carbon-carbon bond-forming process.

## Frequently Asked Questions

### What is the primary purpose of using magnesium in the Grignard reaction with phenyl bromide?

Magnesium acts as a metal reagent that reacts with phenyl bromide to form the phenylmagnesium bromide, a Grignard reagent essential for subsequent nucleophilic addition steps.

### How does phenyl bromide react with magnesium in the Grignard reaction?

Phenyl bromide reacts with magnesium to form phenylmagnesium bromide, which involves the insertion of magnesium into the carbon-bromine bond, creating a highly reactive nucleophile.

### Why is carbon dioxide added after forming the Grignard reagent in this reaction?

Carbon dioxide is added to quench the Grignard reagent, leading to the formation of a phenylcarboxylic acid derivative, typically benzoic acid, upon acid workup.

### What is the significance of using 10 grams of carbon dioxide in this reaction setup?

Using 10 grams of carbon dioxide ensures an excess amount to fully react with the Grignard reagent, driving the formation of the carboxylic acid product and maximizing yield.

### How is the amount of phenyl bromide (1.4555 g) relevant to the stoichiometry of the reaction?

The 1.4555 g of phenyl bromide corresponds to a specific molar amount that determines the theoretical yield of the Grignard reagent and subsequent product, based on molar ratios.

### What role does the amount of magnesium (0.5734 g) play in the reaction efficiency?

The amount of magnesium influences the completeness of Grignard reagent formation; insufficient magnesium can lead to incomplete reaction, while excess ensures full conversion of phenyl bromide.

## What safety precautions should be taken when performing a Grignard reaction with phenyl bromide and carbon dioxide?

Proper safety measures include working in a dry, inert atmosphere (e.g., nitrogen or argon), handling magnesium and organic solvents carefully, and avoiding moisture contact to prevent unwanted reactions or fire hazards.

## What is the expected main product after reaction of phenylmagnesium bromide with carbon dioxide?

The main product is benzoic acid, formed after acid workup of the phenylcarboxylate intermediate generated when the Grignard reagent reacts with carbon dioxide.

# Additional Resources

**Analysis of the Grignard Reaction Utilizing Phenyl Bromide, Carbon Dioxide, and Magnesium: A Detailed Examination**

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Introduction

The Grignard reaction remains one of the most versatile and foundational reactions in organic synthesis, enabling the formation of a wide array of carbon-carbon bonds with precision. In a typical laboratory setup, the reaction involves the formation of a Grignard reagent from an organohalide and magnesium metal, followed by its subsequent reaction with electrophiles such as carbon dioxide to produce carboxylic acids. The specific quantities used—namely 1.4555 grams of phenyl bromide, 10 grams of carbon dioxide, and 0.5734 grams of magnesium—offer an insightful case study into the reaction's stoichiometry, efficiency, and potential yield. This comprehensive review aims to analyze each component's role, calculate theoretical yields, discuss experimental considerations, and interpret the implications of these quantities in the context of synthetic organic chemistry.

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1. The Fundamentals of the Grignard Reaction

1.1 Overview and Significance

The Grignard reaction, first discovered by Victor Grignard in 1900, involves the formation of an organomagnesium halide (Grignard reagent) by the reaction of an alkyl or aryl halide with magnesium metal in an anhydrous solvent, typically diethyl ether or tetrahydrofuran (THF). Once formed, the Grignard reagent acts as a nucleophile, attacking electrophilic centers such as carbonyl groups or carbon dioxide, leading to the formation of alcohols or acids after subsequent hydrolysis.

1.2 Typical Reaction Pathway

The key steps include:

1. Formation of the Grignard reagent:

\[
\text{ArBr} + Mg \rightarrow \text{ArMgBr}
\]

2. Reaction with carbon dioxide:

\[
\text{ArMgBr} + CO_2 \rightarrow \text{ArCO}_2MgBr
\]

3. Acid workup:

\[
\text{ArCO}_2MgBr + H_2O \rightarrow \text{ArCOOH} + MgBr(OH)
\]

The final product, phenylacetic acid in this case, is obtained after acidification.

---

2. Quantitative Analysis of the Reactants

2.1 Phenyl Bromide ($C_6H_5Br$)

- Mass used: 1.4555 grams
- Molecular weight: 157.01 g/mol

Calculation of moles:

\[
\text{Moles of phenyl bromide} = \frac{1.4555\, \text{g}}{157.01\, \text{g/mol}} \approx 0.00927\, \text{mol}

\]

## 2.2 Magnesium (Mg)

- Mass used: 0.5734 grams
- Atomic weight: 24.305 g/mol

Calculation of moles:

$$
\text{Moles of Mg} = \frac{0.5734\, \text{g}}{24.305\, \text{g/mol}} \approx 0.0236\, \text{mol}
$$

## 2.3 Carbon Dioxide ($CO_2$)

- Mass used: 10 grams
- Molecular weight: 44.01 g/mol

Calculation of moles:

$$
\text{Moles of CO}_2 = \frac{10\, \text{g}}{44.01\, \text{g/mol}} \approx 0.2273\, \text{mol}
$$

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# 3. Stoichiometric Considerations and Reactant Ratios

## 3.1 Expected Molar Ratios

The overall process involves:

- 1 mol of phenyl bromide reacting with 1 mol of magnesium to produce 1 mol of phenylmagnesium bromide.
- 1 mol of phenylmagnesium bromide reacting with 1 mol of $CO_2$ to produce phenylacetic acid after hydrolysis.

Ideal molar ratios:

- Phenyl bromide : Mg : $CO_2$ = 1 : 1 : 1

Given quantities:

- Phenyl bromide: 0.00927 mol
- Mg: 0.0236 mol (excess)
- $CO_2$: 0.2273 mol (excess)

Implication: Magnesium is in excess relative to phenyl bromide, which favors complete formation of phenylmagnesium bromide. Carbon dioxide is also in large excess, ensuring complete carboxylation of the Grignard reagent.

### 3.2 Reagent Excess and Reaction Efficiency

Having excess magnesium and $CO_2$ is standard practice to push the reaction toward completion. Excess magnesium compensates for any surface passivation or incomplete activation, while excess $CO_2$ ensures full conversion of the Grignard reagent to the carboxylate intermediate.

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## 4. Theoretical Yield Calculations

### 4.1 Formation of Phenylmagnesium Bromide

- Theoretical maximum: 0.00927 mol
- Mass of phenylacetic acid produced: Assuming 100% yield, the molar mass of phenylacetic acid ($C_8H_8O_2$) is approximately 136.15 g/mol.

$$
\text{Mass of phenylacetic acid} = 0.00927\, \text{mol} \times 136.15\, \text{g/mol} \approx 1.262\, \text{g}
$$

### 4.2 Expected Yield

In practical laboratory settings, yields typically range from 70% to 90%, depending on purity, reaction conditions, and procedural efficiency.

- Estimated yield range:

- 70% yield: $\approx 0.70 \times 1.262\, \text{g} \approx 0.883\, \text{g}$
- 90% yield: $\approx 1.136\, \text{g}$

This indicates that, under ideal conditions, approximately 0.88 to 1.14 grams of phenylacetic acid could be obtained from the given quantities.

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## 5. Experimental Considerations and Potential Challenges

### 5.1 Reaction Conditions

- Anhydrous environment: The formation of Grignard reagents requires strictly anhydrous conditions to prevent hydrolysis.
- Solvent selection: Diethyl ether or THF are standard solvents, providing a suitable medium for the reaction.
- Temperature control: Typically, reactions are carried out at room temperature or slightly below to minimize side reactions.

### 5.2 Reaction Kinetics and Completion

- The surface area and activation state of magnesium influence the rate of Grignard formation.
- Adequate stirring and gentle heating can accelerate the formation of phenylmagnesium bromide.
- The addition of phenyl bromide to magnesium in the solvent must be controlled to prevent exothermic runaway.

### 5.3 Challenges in $CO_2$ Reaction

- Ensuring uniform $CO_2$ distribution in the reaction mixture is crucial.
- $CO_2$ gas bubbling can be inefficient if not properly managed.
- The reaction's exothermic nature necessitates controlled addition and temperature monitoring.

### 5.4 Side Reactions and Byproducts

- Formation of biphenyl via coupling of phenyl radicals or magnesium insertion reactions.
- Hydrolysis of the Grignard reagent if moisture ingress occurs.
- Incomplete reaction leading to residual starting halide.

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## 6. Analytical Techniques and Product Verification

### 6.1 Spectroscopic Analysis

- NMR spectroscopy: To confirm the formation of phenylacetic acid, characteristic aromatic and carboxylic acid signals can be observed.
- Infrared (IR) spectroscopy: The presence of a broad O-H stretch (~2500–3300 $cm^{-1}$) and C=O stretch (~1700 $cm^{-1}$) confirms carboxylic acid formation.
- Mass spectrometry: To verify the molecular weight and purity of the product.

### 6.2 Purification Methods

- Acidic workup followed by extraction.
- Recrystallization from appropriate solvents to purify phenylacetic acid.

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7. Broader Implications and Applications

7.1 Synthetic Utility of Phenylacetic Acid

Phenylacetic acid serves as a precursor in pharmaceutical synthesis, perfume manufacturing, and as an intermediate in the production of various organic compounds.

7.2 Scalability and Industrial Relevance

Understanding the stoichiometry and efficiency of this reaction informs scale-up processes, especially in pharmaceutical manufacturing where yield optimization is critical.

7.3 Environmental and Safety Considerations

- Proper handling of magnesium and diethyl ether, which are flammable and reactive.
- Efficient reaction conditions reduce waste and improve overall sustainability.

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8. Conclusion

The reaction setup involving 1.4555 grams of phenyl bromide, 10 grams of carbon dioxide, and 0.5734 grams of magnesium exemplifies fundamental principles of the Grignard reaction, balancing reagent quantities, reaction efficiency, and product yield. Quantitative analysis reveals that, theoretically, up to approximately 1.14 grams of phenylacetic acid could be synthesized under ideal conditions, with practical yields potentially slightly lower due to procedural losses. This case study underscores the importance of precise stoichiometry, rigorous experimental

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