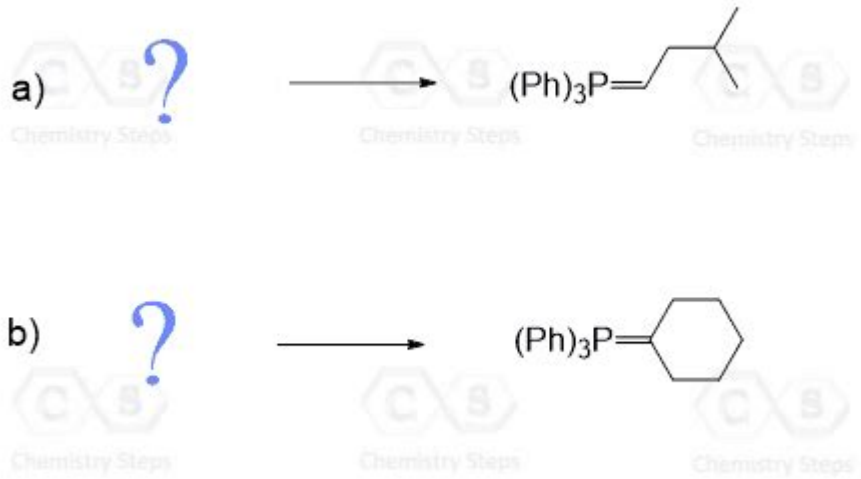
Wittig Reaction Practice Problems



Wittig reaction practice problems are essential in mastering this significant organic chemistry reaction. The Wittig reaction is a powerful method for forming alkenes by reacting an aldehyde or ketone with a phosphonium ylide. Understanding the mechanisms, predicting products, and applying the reaction to various practice problems can greatly enhance one's grasp of organic synthesis. In this article, we will delve into the details of the Wittig reaction, review its mechanism, and provide various practice problems to bolster your understanding.

Overview of the Wittig Reaction

The Wittig reaction was developed by Georg Wittig, who was awarded the Nobel Prize in Chemistry in 1979 for this work. It plays a crucial role in organic synthesis, particularly in the formation of alkenes from carbonyl compounds. The general reaction can be summarized as follows:

1. A phosphonium ylide reacts with an aldehyde or ketone.
2. This results in the formation of an alkene and a byproduct, which is typically a phosphine oxide.

Mechanism of the Wittig Reaction

The mechanism of the Wittig reaction involves several key steps:

1. Formation of Phosphonium Ylide: The reaction begins with the generation of a phosphonium ylide from a phosphonium salt (R3P+X−) and a strong base (e.g., n-butyllithium or sodium hydride).

$$
R_3P^+X^- + \text{Base} \rightarrow R_2C=PR_3 + HX
$$

2. Nucleophilic Attack: The ylide acts as a nucleophile and attacks the carbonyl carbon of the aldehyde or ketone.

$$
R_2C=PR_3 + R'CHO \rightarrow R_2C(OH)PR_3^-
$$

3. Formation of the Alkene: The intermediate undergoes a rearrangement to form the alkene and yields a phosphine oxide as a byproduct.

$$
R_2C(OH)PR_3^- \rightarrow R_2C=CHR' + R_3P=O
$$

Understanding this mechanism is crucial for solving practice problems effectively.

Types of Wittig Reactions

There are two main types of Wittig reactions:

1. Stabilized Ylides: These ylides contain electron-withdrawing groups, which stabilize the ylide and can lead to the formation of E/Z isomers.

2. Unstabilized Ylides: These ylides do not have electron-withdrawing groups and typically yield only one stereochemical outcome.

Key Considerations in Wittig Reactions

- Selectivity: The stereochemistry of the product can be influenced by the nature of the ylide used. Stabilized ylides tend to favor the formation of Z-alkenes, while unstabilized ylides favor E-alkenes.

- Solvent Effects: The choice of solvent can also impact the reaction outcome and selectivity.

- Functional Group Compatibility: Some functional groups can interfere with the reaction, so it is essential to consider the substrate's compatibility.

Practice Problems

Now that we have covered the fundamentals, let's dive into some practice problems to test your understanding of the Wittig reaction.

Problem Set 1: Predicting Products

1. Given the following reaction, predict the major product:

$$
\text{Ph}_3P=CH_2 + \text{C}_6H_5CHO \rightarrow ?
$$

2. For the reaction between the following compounds, identify the product:

$$
\text{Ph}_3P=CHCOOEt + \text{C}_6H_5C(O)CH_3 \rightarrow ?
$$

3. Using the ylide generated from benzyltriphenylphosphonium chloride and sodium hydride, react it with cyclopentanone. What is the expected product?

$$
\text{Ph}_3P^+CH_2C_6H_5 + \text{C}_5H_{10}O \rightarrow ?
$$

Problem Set 2: Mechanism Understanding

1. Write the complete mechanism for the reaction of benzaldehyde with triphenylphosphonium ylide.

2. Explain why the reaction of a stabilized ylide with an aldehyde might yield a mixture of E/Z isomers.

3. Describe what happens during the formation of the alkene in the Wittig reaction. What factors influence the stereochemistry of the product?

Problem Set 3: Application of Wittig Reaction

1. Design a synthetic route to produce 1-phenylbut-1-ene starting from benzaldehyde using the Wittig reaction. Include all necessary reagents.

2. Given a target molecule, outline a synthetic pathway using the Wittig reaction to introduce a double bond. Explain your reasoning for each step.

3. Discuss the limitations of the Wittig reaction in organic synthesis. What alternatives could be employed when the Wittig reaction is not suitable?

Answers and Explanations

To maximize learning, here are the answers to the practice problems:

Answers to Problem Set 1

1. The major product is (E)-1,2-diphenylethylene.
2. The product would be (E)-3-phenyl-2-butenedioate.
3. The expected product is 1-phenylcyclopentene.

Answers to Problem Set 2

1. The mechanism involves the nucleophilic attack of the ylide on the carbonyl carbon, followed by rearrangement to form the alkene and phosphine oxide.
2. Stabilized ylides can result in different conformations due to steric interactions, leading to a mixture of E/Z isomers.
3. The alkene forms through a [2 + 2] cycloaddition-like mechanism, where the stereochemistry is influenced by the geometry of the ylide and the carbonyl compound.

Answers to Problem Set 3

1. A possible route is to first convert benzaldehyde to the ylide, then react it with 1-bromobutane to form 1-phenylbut-1-ene.
2. The pathway may involve starting from an alkene, using the Wittig reaction to introduce a double bond, followed by further transformations.
3. Limitations include sensitivity to functional groups and potential side reactions. Alternatives like the Horner-Wadsworth-Emmons reaction can often be used.

Conclusion

The Wittig reaction is a cornerstone of organic synthesis, enabling the formation of alkenes from carbonyl compounds. Through practice problems, students can solidify their understanding of this reaction's mechanisms, applications, and limitations. By mastering **wittig reaction practice problems**, chemists can enhance their synthetic strategy toolbox, paving the

way for innovative organic chemistry solutions.

Frequently Asked Questions

What is the Wittig reaction primarily used for?

The Wittig reaction is primarily used to convert carbonyl compounds into alkenes through the reaction with phosphonium ylides.

What type of reaction mechanism does the Wittig reaction follow?

The Wittig reaction follows a nucleophilic substitution mechanism where the phosphonium ylide acts as a nucleophile attacking the carbonyl carbon.

What are common starting materials for the Wittig reaction?

Common starting materials include aldehydes or ketones as the carbonyl compounds and phosphonium salts to generate the ylides.

What is the role of the phosphonium ylide in the Wittig reaction?

The phosphonium ylide serves as a nucleophile that attacks the electrophilic carbonyl carbon, forming an alkene and a phosphine oxide.

Can the Wittig reaction be used to create stereospecific alkenes?

Yes, the Wittig reaction can be used to create stereospecific alkenes, allowing for the formation of either E or Z isomers depending on the configuration of the ylide.

What factors influence the selectivity of the Wittig reaction?

Selectivity in the Wittig reaction can be influenced by the electronic and steric properties of the substituents on the ylide and the carbonyl compound.

What are some common side reactions that can occur during the Wittig reaction?

Common side reactions include the formation of byproducts from the decomposition of the ylide or competitive reactions with solvents or other nucleophiles.

How can you generate a phosphonium ylide for the Wittig reaction?

A phosphonium ylide can be generated by deprotonating a phosphonium salt using a strong base, such as butyllithium or sodium hydride.

What are the limitations of the Wittig reaction?

Limitations of the Wittig reaction include the potential for low yields, formation of side products, and difficulties in synthesizing certain ylides, especially those with sterically hindered groups.

How do you determine the E/Z configuration of the alkene produced from a Wittig reaction?

The E/Z configuration can be determined using the Cahn-Ingold-Prelog priority rules based on the substituents attached to the double bond formed in the Wittig reaction.

Wittig Reaction Practice Problems

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