80) What Is The Major Organic Product That Resultswhen 1-heptyne Is Treated With 2 Equivalents Of HBr?A)

80) What Is The Major Organic Product That Resultswhen 1-heptyne Is Treated With 2 Equivalents Of HBr?A)

When 1-heptyne, a terminal alkyne, is treated with two equivalents of hydrobromic acid (HBr), the reaction proceeds through a well-understood addition mechanism, ultimately leading to the formation of a significant organic product. This process involves the addition of hydrogen bromide across the triple bond, transforming it into a dibromoalkane. The major organic product resulting from this reaction is 1,1-dibromoheptane.

Understanding this transformation requires a comprehensive grasp of alkyne reactivity, the nature of hydrohalic acid additions, and the factors influencing regioselectivity. This article delves into the reaction pathway, mechanisms, and key points to understand why 1,1-dibromoheptane is the major product when 1-heptyne reacts with two equivalents of HBr.

Overview of 1-Heptyne and Its Reactivity

Structure and Properties of 1-Heptyne

- Chemical formula: C7H12
- Structural features: Terminal alkyne with a triple bond between the first and second carbon atoms.
- Reactivity: Alkynes are characterized by their high reactivity due to the triple bond, which contains a sigma bond and two pi bonds. They readily undergo addition reactions with electrophiles such as HBr.

Significance of the Terminal Triple Bond

- The terminal position of the triple bond makes the alkyne more reactive towards electrophilic addition.
- The acidity of the terminal hydrogen (on the carbon bearing the triple bond) influences the reaction pathway, particularly in reactions with acids.

Reaction of 1-Heptyne with HBr: General Principles

Electrophilic Addition to Alkynes

- Alkynes undergo addition reactions similar to alkenes but with different regioselectivity and mechanisms.
- The addition of HBr involves an electrophilic attack on the electron-rich triple bond.

Stepwise Addition of HBr

- First, HBr adds across the triple bond to form a vinyl bromide intermediate.
- With excess HBr (two equivalents), this process continues, leading to a dibrominated product.

Role of Equivalents of HBr

- One equivalent of HBr generally results in mono-bromination.
- Two equivalents lead to dibromination, specifically adding bromine atoms to the carbons previously involved in the triple bond.

Mechanism of the Addition Reaction

Step 1: Formation of the Vinyl Bromide

- The initial addition involves the electrophilic H+ attacking the terminal carbon of the triple bond.
- A carbocation intermediate forms, stabilized by the alkyl chain.
- Bromide ion (Br-) then adds to the carbocation, resulting in a vinyl bromide.

Step 2: Second Addition of HBr

- The vinyl bromide undergoes a second addition of HBr.
- The addition occurs across the double bond formed after the first addition.
- The second bromine atom attaches to the same carbon that initially received the proton, leading to a dihalogenated product.

Markovnikov's Rule and Regioselectivity

- The addition of HBr proceeds following Markovnikov's rule, favoring addition where the proton adds to the carbon with more hydrogens.
- In terminal alkynes, the proton typically adds to the terminal carbon, leading to specific regioisomers.

Major Organic Product: 1,1-Dibromoheptane

Structure and Identification

- The major product formed is 1,1-dibromoheptane, characterized by two bromine atoms attached to the same terminal carbon (carbon-1).
- Structural formula: CH3–CH2–CH2–CH2–CH2–CH2–CBr2

Why 1,1-Dibromoheptane Is the Major Product

- The reaction favors addition at the terminal alkyne carbon, especially under conditions with excess HBr.
- The first addition of HBr creates a vinyl bromide intermediate.
- The second addition occurs at the same carbon, leading to geminal dibromide formation.

Factors Influencing Product Formation

- Regioselectivity: Due to Markovnikov's rule, the proton adds to the terminal carbon, and bromide adds to the more substituted carbon.
- Reaction conditions: Excess HBr pushes the reaction toward dibromination.
- Stability of intermediates: The formation of a stable carbocation intermediate favors addition at the terminal carbon.

Alternative Possible Products and Their Formation

1,2-Dibromoheptane (Less Major)

- Formed if bromide adds to the internal carbon after the initial addition.
- Less favored under typical conditions due to regioselectivity.

Other Possible Side Reactions

- Polymerization or over-addition leading to complex mixtures.
- Addition of HBr to form vinyl bromides that may undergo further reactions.

Practical Applications and Significance

Industrial Relevance

- Synthesis of brominated alkanes used in pharmaceuticals, agrochemicals, and material sciences.
- Understanding addition reactions helps in designing pathways for complex molecule synthesis.

Educational Importance

- Demonstrates fundamental principles of organic addition reactions.
- Clarifies regioselectivity and stereochemistry in alkyne reactions.

Key Takeaways for Organic Chemists

- The addition of 2 equivalents of HBr to 1-heptyne yields 1,1-dibromoheptane as the major product.
- Reaction proceeds via electrophilic addition following Markovnikov's rule.
- The process exemplifies the reactivity of terminal alkynes with electrophiles.

Summary

In conclusion, when 1-heptyne reacts with two equivalents of hydrobromic acid (HBr), the major organic product formed is 1,1-dibromoheptane. This transformation involves a two-step addition mechanism where the triple bond first adds HBr to form a vinyl bromide, followed by a second addition leading to a geminal dibromide. The regioselectivity and reaction conditions favor addition at the terminal carbon, resulting in the formation of 1,1-dibromoheptane, a key intermediate in organic synthesis. Understanding this reaction provides insight into alkyne reactivity, electrophilic addition mechanisms, and the principles governing regioselective transformations in organic chemistry.

Keywords: 1-heptyne, HBr addition, dibromoalkane, electrophilic addition, regioselectivity, Markovnikov's rule, organic synthesis, terminal alkyne, 1,1-dibromoheptane, alkyne reactivity, organic reactions

Frequently Asked Questions

What is the major organic product formed when 1-heptyne reacts with 2 equivalents of HBr?

The major product is 1-bromo-2-heptene, resulting from the anti-Markovnikov addition across the triple bond, converting it to a dibromoalkene.

How does the addition of HBr to 1-heptyne proceed in terms of regioselectivity?

The addition occurs via anti-Markovnikov orientation, meaning the bromine adds to the terminal carbon, resulting in a vinyl bromide.

What is the significance of using 2 equivalents of HBr in the reaction with 1-heptyne?

Using 2 equivalents ensures the complete addition of two bromine atoms across the triple bond, converting it into a dibrominated alkene.

What type of reaction mechanism is involved when 1-heptyne reacts with HBr?

The reaction proceeds via an electrophilic addition mechanism, where HBr adds across the triple bond to form a vinyl bromide intermediate.

Can the reaction of 1-heptyne with 2 equivalents of HBr be controlled to yield a specific product?

Yes, reaction conditions such as temperature and solvent can influence the selectivity, but generally, 2 equivalents of HBr lead to dibromoalkenes as the major product.

What are the safety considerations when handling HBr in organic reactions?

HBr is highly corrosive and toxic; proper protective equipment, such as gloves and goggles, and working in a fume hood are essential to ensure safety.

Additional Resources

Understanding the Reaction of 1-Heptyne with 2 Equivalents of HBr: Major Organic Product and Its Significance

In the realm of organic chemistry, the transformations of alkynes such as 1-heptyne with halogen acids like hydrobromic acid (HBr) are fundamental reactions that reveal much about molecular reactivity, regioselectivity, and the mechanisms governing addition processes. When 1-heptyne, a terminal alkyne, interacts with two equivalents of HBr, it undergoes a two-step addition process culminating in a specific, predictable product. This article aims to delve into the detailed chemistry behind this reaction, explore the nature of the major organic product formed, and analyze its significance within broader synthetic applications.

Introduction to 1-Heptyne and Its Reactivity

1.1. Structural and Electronic Characteristics of 1-Heptyne

1-heptyne is a linear, terminal alkyne with the molecular formula C7H12. Its structure features a triple bond between the first and second carbon atoms, making it an unsaturated hydrocarbon with distinctive reactivity. The terminal nature of the alkyne means that the triple bond is at the end of the carbon chain, with a hydrogen atom attached to the carbon of the triple bond (the terminal carbon).

The electronic configuration of the triple bond involves a sigma bond and two pi bonds, rendering the alkyne electron-rich and susceptible to nucleophilic addition reactions. The acidity of the terminal hydrogen (pKa ≈ 25) is higher than typical alkanes but lower than alcohols, which influences how it reacts with electrophiles like HBr.

1.2. General Reactivity of Alkynes with Hydrogen Halides

Alkynes tend to undergo electrophilic addition reactions with hydrogen halides (HX, where X = Cl, Br, I). These additions are characterized by their regioselectivity and the possibility of multiple additions, depending on the amount of HX used. In the case of terminal alkynes, the addition of HX typically proceeds via a Markovnikov mechanism, where the proton adds to the carbon with more hydrogens, and the halide attaches to the more substituted carbon after the initial protonation.

Reaction of 1-Heptyne with Hydrobromic Acid (HBr)

2.1. Overview of the Addition Process

When 1-heptyne is treated with 2 equivalents of HBr, the reaction proceeds through a two-step addition process:

- First addition: Protonation of the triple bond, followed by halide addition, yields a vinyl bromide (alkenyl bromide).
- Second addition: The process repeats on the newly formed alkene, leading to a geminal dibromide (a molecule with two bromine atoms attached to the same carbon).

2.2. Step-by-Step Mechanism

- Step 1: Protonation of the terminal alkyne occurs at the terminal carbon, generating a carbocation intermediate stabilized by the adjacent carbon chain. The electrophilic H+ from HBr adds to the terminal carbon, forming a carbocation.

- Step 2: Bromide ion (Br−) then attacks the carbocation, giving an organobromide intermediate—specifically, an alkene with a bromine atom attached.

- Step 3: The second equivalent of HBr reacts with this alkene, again via electrophilic addition. Because the alkene is now more substituted than the original alkyne, the addition proceeds with regioselectivity favoring the formation of the more stable carbocation.

- Step 4: Bromide attacks the carbocation formed during the second addition, resulting in a vicinal dibromide, with both bromines attached to the same carbon atom (geminal dibromide).

Major Organic Product: 1,1-Dibromoheptane

3.1. Structural Identity of the Product

The key product resulting from the complete two-step addition of HBr to 1-heptyne is 1,1-dibromoheptane. Its structure can be described as:

- A linear seven-carbon chain.
- Two bromine atoms attached to the first carbon (the terminal carbon originally bearing the triple bond).

3.2. Structural Explanation

The product is a geminal dibromide, meaning both bromines are attached to the same carbon atom. The overall transformation involves converting the terminal alkyne into a saturated alkyl chain with two bromines on the terminal carbon, effectively replacing the triple bond with a dibrominated methyl group.

3.3. Chemical Formula and Nomenclature

- The molecular formula of the product is C7H14Br2.
- Its IUPAC name is 1,1-dibromoheptane.

Mechanistic Rationale Behind the Formation of 1,1-Dibromoheptane

4.1. Markovnikov Addition and Regioselectivity

The addition of HBr to alkynes follows Markovnikov’s rule—where the proton adds to the carbon with more hydrogens, and the halide attaches to the more substituted carbon or, in terminal alkynes, to the terminal carbon. Due to the acidity of the terminal hydrogen and the stability of the carbocation intermediate, the initial addition favors the terminal carbon.

4.2. Formation of Vinyl Bromide Intermediate

The first equivalent of HBr adds across the triple bond, resulting in a vinyl bromide intermediate, specifically 1-bromo-1-heptene. This intermediate is characterized by a double bond between carbons 1 and 2, with a bromine attached to carbon 1.

4.3. Second Addition and Complete Saturation

Adding a second equivalent of HBr to the vinyl bromide leads to the addition across the double bond, with the proton again adding to the carbon bearing more hydrogens, and bromide attacking the carbocation formed during the process. This results in the formation of 1,1-dibromoheptane, with both bromines on the terminal carbon, and the former triple bond fully saturated.

Significance of the Reaction and Its Synthetic Applications

5.1. Synthetic Utility of Dibromides

The formation of geminal dibromides like 1,1-dibromoheptane is valuable in organic synthesis for several reasons:

- Precursor to Organometallic Reagents: Dibromides can be converted into organomagnesium or organolithium compounds, which are key intermediates in complex molecule construction.
- Functional Group Transformations: They serve as starting points for further functionalization via nucleophilic substitution, elimination, or coupling reactions.
- Building Blocks for Cyclizations: The presence of two halogens on a single carbon allows for intramolecular reactions, including cyclizations, to synthesize cyclic compounds.

5.2. Understanding Regioselectivity and Stereochemistry

The reaction illustrates the importance of regioselectivity in electrophilic addition to alkynes. It highlights that terminal alkynes tend to undergo Markovnikov addition with electrophiles, leading predominantly to the geminal dibromide. Such understanding is crucial when designing synthesis pathways that require specific regio- or stereochemical outcomes.

5.3. Broader Implications in Organic Chemistry

Analyzing this reaction deepens insights into the mechanisms of alkyne halogenation, the stability of carbocation intermediates, and the influence of electronic factors on reaction pathways. It also underscores the importance of controlling reagent equivalents to dictate the degree of addition—mono or dihalogenation.

Comparison with Other Halogenation Reactions

6.1. Hydrohalogenation vs. Halogenation

While HBr addition to alkynes results in geminal dibromides, other halogen acids like HCl or HI lead to similar or different products depending on their reactivity and the reaction conditions. For example:

- HCl: Typically produces dichlorides, with similar regioselectivity.
- HI: Less common for such additions due to its reactivity and potential for reduction.

6.2. Stereochemistry and Reaction Conditions

The addition reactions are generally syn, meaning the two new substituents add to the same face of the alkyne. Reaction conditions like temperature,

solvent, and the presence of catalysts can influence stereoselectivity, though in the case of terminal alkynes with HBr, the regioselectivity is more prominent.

Conclusion: The Major Organic Product and Its Context

In summary, when 1-heptyne is treated with 2 equivalents of hydrobromic acid, the major organic product formed is 1,1-dibromoheptane. This transformation exemplifies the electrophilic addition mechanism characteristic of alkynes and underscores the importance of reagent stoichiometry in controlling the degree of halogenation. The formation of geminal dibromides as key intermediates or products is significant in synthetic organic chemistry, providing versatile intermediates for further functionalization and complex molecule synthesis.

Understanding the detailed mechanistic pathways, regioselectivity, and stereochemical considerations involved in such reactions is essential for chemists aiming to design efficient synthesis routes. Moreover, the principles gleaned from this reaction extend broadly across organic chemistry, informing strategies for halogenation, functional group manipulation, and the construction of sophisticated molecular architectures.

References:

1. Clayden, Greeves, Warren, and Wothers, Organic

80 What Is The Major Organic Product That Resultswhen 1 Heptyne Is Treated With 2 Equivalents Of Hbr A

80 What Is The Major Organic Product That Resultswhen 1 Heptyne Is Treated With 2 Equivalents Of Hbr A

Related Articles

- A Not-so-skilled Volleyball Player Has A 15% Chance Of Making The Serve, Which Involves Hitting The Ball
- A Young's Interference Experiment Is Performed With Blue-green Argon Laser Light. The Separation Between
- 3. Use Node-Voltage Method To Calculate The Following: A. Find Value Of Vo Across 40

Resistance. B. Find

Back to Home