Vinylcyclohexane Reacts With Three Different Conditions To Give Three Different Products. Draw The Major

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Understanding how vinylcyclohexane reacts under various conditions is fundamental in organic chemistry, especially in the context of synthesizing diverse cyclic compounds. Such reactions demonstrate the versatility of vinylcyclohexane as a substrate and how different reagents, temperature regimes, or catalysts can steer the reaction pathway toward distinct products. This article explores three different conditions under which vinylcyclohexane reacts, the resultant major products, and the mechanistic insights behind these transformations. Visualizing and drawing the major products provides a comprehensive understanding of these reactions, crucial for students and practitioners in organic synthesis.

Introduction to Vinylcyclohexane Reactivity

Vinylcyclohexane is a cyclic alkene featuring a vinyl group attached to a cyclohexane ring. Its structure combines the properties of both cycloalkanes and alkenes, making it a versatile intermediate in various reactions such as addition, elimination, and rearrangements. The nature of these reactions depends heavily on the reaction conditions, including the type of reagents, catalysts, temperature, and solvent.

The three different conditions discussed herein—hydrogenation, electrophilic addition, and oxidative cleavage—highlight the diverse pathways vinylcyclohexane can undergo. Each pathway leads to a distinctly different product, illustrating the importance of controlling reaction conditions for desired outcomes in organic synthesis.

Reaction 1: Hydrogenation of Vinylcyclohexane

Hydrogenation involves the addition of hydrogen (H_2) across a carbon–carbon multiple bond, typically in the presence of a metal catalyst such as palladium, platinum, or nickel.

Reaction Conditions

- Catalyst: Pd/C (palladium on carbon)
- Temperature: Room temperature to mild heating (~25-50°C)

- Pressure: 1-5 atm of hydrogen gas
- Solvent: Usually inert solvents like ethanol or ethyl acetate

Major Product: Cyclohexane

Under these conditions, the vinyl group on vinylcyclohexane is fully saturated, converting the alkene into an alkane. The major product is cyclohexane, a simple saturated ring.

Mechanism Overview

1. Adsorption of vinylcyclohexane onto the metal surface.
2. Dissociation of H_2 into atomic hydrogen on the catalyst.
3. Addition of hydrogen atoms across the double bond.
4. Desorption of the saturated product, cyclohexane.

Drawing the Major Product

The product, cyclohexane, is a six-membered ring with all single bonds:

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Note: When drawing in a detailed structure, cyclohexane can be depicted as a hexagon with bonds between vertices. Remember to indicate that the vinyl group has been fully hydrogenated, removing the double bond.

Reaction 2: Acid-Catalyzed Electrophilic Addition to Vinylcyclohexane

Electrophilic addition reactions involve adding an electrophile across a carbon–carbon double bond. Acid catalysis often facilitates such additions, especially with reagents like H_2SO_4, HBr, or HCl.

Reaction Conditions

- Reagent: Sulfuric acid (H_2SO_4), Hydrobromic acid (HBr), or Hydrochloric acid (HCl)
- Temperature: Ambient or slightly elevated (~25-50°C)
- Catalyst: Proton (H^+) from acid

Major Product: Alkyl Halide or Alcohol Derivative

Depending on the acid used, the reaction yields:
- With HBr or HCl: a halogenated product (e.g., 1-bromocyclohexane)
- With sulfuric acid and water: a hydroxylated product (e.g., cyclohexanol)

In this context, consider addition of HBr, which proceeds via Markovnikov's rule, resulting in the halogen attaching to the more stabilized carbocation.

Mechanism Overview

1. Protonation of the alkene to form a carbocation intermediate.
2. Nucleophilic attack by halide ion (Br^-).
3. Formation of a new C–X bond (X = Cl, Br).

Drawing the Major Product

For HBr addition, the major product is 1-bromocyclohexane, where the bromine is attached to the carbon atom initially bearing the carbocation:

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Note: Draw the cyclohexane ring with a bromine substituent on one carbon, indicating that the addition occurred across the double bond, with the bromine on the more substituted carbon.

Reaction 3: Oxidative Cleavage of Vinylcyclohexane

Oxidative cleavage involves breaking the carbon–carbon double bond and oxidizing the resulting fragments to carbonyl compounds, often using strong oxidants like potassium permanganate ($KMnO_4$) under controlled conditions.

Reaction Conditions

- Oxidant: Potassium permanganate ($KMnO_4$) in aqueous solution
- Temperature: Cold or room temperature
- Acidic or neutral pH: Usually neutral or slightly basic conditions

Major Products: Adipic Acid and Other Dicarboxylic Acids

Oxidative cleavage of vinylcyclohexane leads to ring fragmentation, producing adipic acid (hexanedioic acid) and possibly other dicarboxylic acids depending on reaction conditions.

Mechanism Overview

1. Formation of diol intermediates via initial oxidation.
2. Cleavage of the double bond, breaking the ring into linear fragments.
3. Oxidation of these fragments into carboxylic acids.

Drawing the Major Products

The primary product, adipic acid, is a six-carbon linear dicarboxylic acid:

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HOOC–(CH2)4–COOH
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Note: When drawing adipic acid, depict a chain of six carbons with carboxyl groups at both ends, emphasizing the oxidation and cleavage process that transforms the cyclohexane ring into a linear chain.

Summary and Importance of Reaction Conditions

The reactions of vinylcyclohexane under different conditions exemplify the importance of reaction environment in organic synthesis. By altering catalysts, reagents, temperature, and other parameters, chemists can selectively produce a variety of compounds from a common starting material.

- Hydrogenation under catalytic conditions yields saturated cyclohexane.
- Electrophilic addition with acids introduces halogens or hydroxyl groups.
- Oxidative cleavage with strong oxidants breaks down the ring into linear acids.

Understanding these transformations not only aids in designing synthetic routes but also provides insight into the mechanistic pathways governing organic reactions.

Conclusion

Vinylcyclohexane serves as a prime example of a versatile substrate that can undergo multiple reactions depending on the conditions employed. Drawing the major products of these reactions

enhances comprehension of their mechanisms and outcomes. Mastery of such transformations is essential for advancing in organic chemistry, enabling chemists to synthesize complex molecules efficiently and selectively.

References

- Clayden, Greeves, Warren, and Wothers. Organic Chemistry. Oxford University Press.
- Solomon, Frye. Organic Chemistry. Wiley.
- March, Jerry. Advanced Organic Chemistry. Wiley.
- Organic Reaction Mechanisms, 4th Edition, by I.L. Finar.

Note: For visual clarity, always sketch the cyclic structures and substituents properly, indicating the stereochemistry where relevant. Using molecular models or software can also aid in visualizing these transformations.

Frequently Asked Questions

What are the three different conditions under which vinylcyclohexane reacts to produce three distinct products?

The three conditions typically involve different reagents and reaction environments: (1) hydrogenation leading to cyclohexane derivatives, (2) electrophilic addition or oxidation resulting in substituted products, and (3) radical or elimination conditions producing cyclohexene derivatives.

How does hydrogenation of vinylcyclohexane differ from its oxidation in terms of the major product?

Hydrogenation adds hydrogen across the double bond, converting vinylcyclohexane into cyclohexane derivatives, while oxidation introduces oxygen functionalities, leading to products such as cyclohexanol or cyclohexanone, depending on the oxidizing agent used.

What is the major product when vinylcyclohexane reacts under radical conditions?

Under radical conditions, the major product is typically a cyclohexane ring with a substituted side chain, such as a cyclohexyl radical addition product, often resulting in cyclohexane derivatives with additional substituents depending on the radical source.

Can you describe the major product formed when

vinylcyclohexane undergoes electrophilic addition reactions?

Electrophilic addition to the double bond of vinylcyclohexane generally yields a cyclohexane ring with a new substituent attached at the former double bond position, such as a halogen or a hydrogen halide, depending on the electrophile used.

How would you draw the major product when vinylcyclohexane reacts under conditions favoring elimination?

Under elimination conditions, the major product is typically cyclohexene with a side chain derived from the original vinyl group, reflecting the removal of elements like HCl or HBr, leading to an unsaturated cyclohexene derivative.

Additional Resources

Vinylcyclohexane Reacts Under Three Different Conditions to Yield Three Distinct Products: An In-Depth Analysis

Vinylcyclohexane is a versatile organic compound that exemplifies the complexity and richness of carbocyclic chemistry. Its reactivity under various conditions underscores fundamental principles in organic synthesis, especially in the realm of electrophilic additions, radical mechanisms, and rearrangement reactions. This comprehensive review explores how vinylcyclohexane, when subjected to three distinct reaction conditions, produces three different products, highlighting the underlying mechanisms, experimental nuances, and implications for synthetic strategy.

Introduction to Vinylcyclohexane: Structure and Significance

Vinylcyclohexane is a cyclic compound consisting of a cyclohexane ring bonded to a vinyl group (–CH=CH_2). Its molecular formula is C8H14, and it features a combination of saturated and unsaturated regions, which imparts a diverse reactivity profile. The conjugated or conjugation-like behavior between the vinyl group and the cyclohexane ring makes it a compelling substrate for various transformations.

Key features include:

- The vinyl group provides a site for addition reactions, radical processes, and rearrangements.
- The cyclohexane ring offers conformational flexibility, influencing regioselectivity and stereoselectivity.
- The molecule can undergo a variety of reactions depending on conditions such as temperature, reagents, catalysts, and solvents.

Understanding how these factors influence reactivity is essential for predicting and controlling product formation.

Reaction Conditions and Their Impact on Product Formation

The three primary reaction conditions explored are:

1. Hydrogenation under catalytic conditions
2. Electrophilic addition with halogens (e.g., Br_2 or Cl_2)
3. Radical-mediated reactions using peroxides or UV light

Each condition engages different mechanistic pathways, leading to unique products. Below, we delve into each reaction scenario with detailed mechanistic insights, experimental protocols, and product analysis.

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1. Hydrogenation of Vinylcyclohexane: Producing Cyclohexane Derivative

Reaction Overview

Hydrogenation involves the addition of hydrogen (H_2) across unsaturated bonds, typically facilitated by a metal catalyst such as palladium (Pd), platinum (Pt), or nickel (Ni). When vinylcyclohexane is hydrogenated under suitable conditions, the vinyl group is transformed into a saturated ethyl group, resulting in a cyclohexane derivative.

Mechanism Details

- Step 1: Adsorption
Vinylcyclohexane adsorbs onto the catalytic surface, aligning the π-bond with the metal.

- Step 2: Hydrogen Activation
H_2 molecules dissociate on the metal surface to generate atomic hydrogen.

- Step 3: Addition
Atomic hydrogen adds across the double bond in a stepwise manner, saturating the vinyl group.

- Step 4: Desorption
The fully hydrogenated product, cyclohexane with an ethyl substituent, desorbs from the catalyst surface.

Expected Product

- Major Product: Ethylcyclohexane
The vinyl group is converted into an ethyl group attached to the cyclohexane ring.

Experimental Conditions

- Catalyst: Pd/C or PtO_2
- Pressure: 1-10 atm H_2
- Temperature: Room temperature to 50°C
- Solvent: Ethanol or ethyl acetate
- Duration: 2–6 hours

Significance and Applications

- Such hydrogenation reactions are fundamental in refining processes, where unsaturated hydrocarbons are saturated.
- The product, ethylcyclohexane, can serve as a starting material for further functionalization or as an intermediate in pharmaceuticals and fine chemicals.

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2. Electrophilic Halogenation: Formation of Halogenated Cyclohexane Derivatives

Reaction Overview

Electrophilic addition of halogens (e.g., Br_2 or Cl_2) to vinylcyclohexane involves addition across the alkene bond. This reaction proceeds via a halonium intermediate, ultimately leading to halogenated products.

Mechanism Details

- Step 1: Formation of Halonium Ion
The π-electrons of the vinyl group attack the halogen molecule (Br_2 or Cl_2), forming a cyclic halonium ion.

- Step 2: Nucleophilic Attack
A halide ion (Br^- or Cl^-) attacks the more accessible carbon of the halonium ion, leading to anti addition.

- Step 3: Product Formation
The result is a vicinal dihalide attached to the cyclohexane ring.

Product Specifics

Depending on reaction conditions, regioselectivity, and steric factors, the major product is:

- 1,2-Dihalocyclohexane derivatives with the halogens added across the former double bond.

For example:

- 1,2-Dibromocyclohexane (if Br_2 is used)
- 1,2-Dichlorocyclohexane (if Cl_2 is used)

Reaction Conditions

- Reagents: Br_2 or Cl_2
- Solvent: Carbon tetrachloride (CCl_4) or dichloromethane (DCM)
- Temperature: Room temperature
- Reaction time: 30 min to 2 hours
- Light: Sometimes reactions are performed in the dark to prevent radical pathways, but UV light can be employed for radical initiation.

Mechanistic Variations and Side Products

- Under radical conditions, side reactions such as radical addition or polymerization may occur.
- In some cases, halogenation at allylic or vinylic positions (allylic halogenation) can compete, leading to a mixture of products.

Significance in Synthesis

- Halogenated cyclohexanes serve as intermediates for further substitution reactions, nucleophilic displacement, or as building blocks for complex molecules.
- They are also valuable in studying stereochemistry and regioselectivity in addition reactions.

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3. Radical Addition Using Peroxides or UV Light: Formation of Cyclohexyl Derivatives

Reaction Overview

Radical reactions are initiated by peroxides or UV light, leading to the addition of radicals across unsaturated bonds. Vinylcyclohexane under radical conditions can undergo additions that lead to cyclohexyl radicals and subsequent hydrogen or other radical additions, resulting in products different from those obtained via ionic pathways.

Mechanism Details

- Step 1: Radical Initiation
Peroxides decompose under heat or UV light to generate radical species (e.g., tert-butoxy radicals).

- Step 2: Radical Addition
The radical adds to the vinyl group, forming a cyclohexyl radical intermediate.

- Step 3: Propagation
The radical intermediate reacts with another molecule (e.g., H_2, or another radical source) to stabilize, forming a new covalent bond.

- Step 4: Termination
Radical coupling results in the formation of the final product.

Possible Products

Depending on the radical source:

- Hydrogen radical addition:
Produces a cyclohexane derivative with a saturated side chain (e.g., cyclohexane with an ethyl group).

- Alkyl radical addition:
Leads to alkylated cyclohexane derivatives, with possible chain elongation or substitution.

- Addition of other radicals (e.g., oxygen or halogen):
Can produce cyclohexanol, cyclohexyl halides, or other functionalized derivatives.

Reaction Conditions

- Radical initiator: Benzoyl peroxide, AIBN, or UV light
- Solvent: Toluene, benzene, or other inert solvents
- Temperature: 80–150°C (for peroxide decomposition)
- Reaction time: Several hours depending on the radical source

Mechanistic Nuances

- Radical reactions often exhibit less regioselectivity compared to ionic processes.
- Stereoselectivity can be influenced by the conformational preferences of the cyclohexane ring.
- Radical chain reactions can lead to complex mixtures, requiring careful purification.

Applications and Significance

- These reactions are valuable in polymer chemistry and the synthesis of complex molecules.
- Radical pathways enable functionalization at otherwise inert positions.
- They also provide insights into reaction kinetics and radical stability.

Comparison and Summary of the Three Products

Reaction Condition	Major Product	Structural Features	Key Mechanistic Pathway	Significance
Hydrogenation	Ethylcyclohexane	Saturated, ethyl substituent	Ionic addition of H_2 across C=C	Industrial solvent, precursor for further synthesis
Halogenation	1,2-Dihalocyclohexane	Vicinal dihalide	Electrophilic halogen addition via halonium ion	Intermediate in organic synthesis and stereochemical studies

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