What Is The Major Product Formed Upon Treatment Of (R) 1-bromo-4-methylhexane With Sodium Cyanide?

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When exploring organic reaction mechanisms, understanding how different reagents interact with various compounds is essential. One intriguing example is the reaction between (R)-1-bromo-4-methylhexane and sodium cyanide. This reaction is a classic demonstration of nucleophilic substitution, particularly the SN2 mechanism, which results in the formation of a new carbon-nitrogen bond. The major product formed in this process provides insight into stereochemistry, reaction pathways, and the influence of substituents on reactivity.

In this comprehensive article, we will delve into the details of the reaction, analyze the stereochemical outcomes, and explore the significance of the product formed upon treatment of (R)-1-bromo-4-methylhexane with sodium cyanide. By the end, you will have a clear understanding of the reaction mechanism, the major product, and its importance in organic synthesis.

Understanding the Reactants: (R)-1-bromo-4-methylhexane and Sodium Cyanide

Before examining the reaction pathway, it is essential to understand the nature of the reactants involved.

Structure of (R)-1-bromo-4-methylhexane

- Molecular formula: C7H15Br
- Structure overview: It is a six-carbon straight chain with a bromine atom attached to the first carbon and a methyl group attached to the fourth carbon.
- Stereochemistry: The (R) configuration indicates a specific spatial arrangement at the chiral center (carbon-1), which influences the reaction's stereochemical outcome.

Structural features:

- The main chain: hexane (six carbons)
- Substituents:
- Bromine atom at carbon-1
- Methyl group at carbon-4
- Chirality at carbon-1: The (R) configuration denotes the stereochemistry according to Cahn-Ingold-Prelog rules.

Sodium Cyanide (NaCN)

- Nature: A strong nucleophile containing the cyanide ion (CN-)
- Role in reactions: Typically involved in nucleophilic substitution reactions, especially SN2 mechanisms with primary or methyl halides.

Reaction Mechanism: Nucleophilic Substitution (SN2)

The reaction of (R)-1-bromo-4-methylhexane with sodium cyanide primarily proceeds via an SN2

mechanism, which involves a one-step bimolecular nucleophilic substitution.

Key Features of SN2 Reactions

- Concerted process: Bond formation and bond cleavage occur simultaneously.
- Backside attack: The nucleophile attacks the electrophilic carbon from the side opposite to the leaving group.
- Stereochemistry: Results in inversion of configuration at the chiral center (Walden inversion).
- Substrate preference: Favored with primary halides, like (R)-1-bromo-4-methylhexane.

Step-by-step Mechanism

1. Nucleophile approach: The cyanide ion (CN-) approaches the electrophilic carbon (carbon-1) from the side opposite to the bromine atom.
2. Transition state formation: A pentavalent transition state develops where the carbon is partially bonded to both the leaving group (Br) and the nucleophile (CN).
3. Leaving group departure: Bromide ion (Br-) departs, while the cyanide ion forms a new bond with the carbon.
4. Product formation: The resulting molecule is (S)-1-cyano-4-methylhexane, due to inversion of stereochemistry.

Major Product: (S)-1-Cyano-4-methylhexane

The primary outcome of this nucleophilic substitution reaction is the formation of (S)-1-cyano-4-methylhexane, a compound where the cyanide group replaces the bromine atom at carbon-1, and the

stereochemical configuration is inverted.

Stereochemical Implications

- Starting with (R)-1-bromo-4-methylhexane, the SN2 mechanism causes inversion at the chiral center.
- Result: The product is the enantiomer with (S) configuration at carbon-1.
- Significance: Stereochemistry is crucial in pharmaceuticals and chiral synthesis because different enantiomers can have vastly different biological activities.

Structural Characteristics of the Product

- Molecular formula: C7H14N
- Functional group: Nitrile (cyano group, –C□N)
- Configuration: (S)-configuration at the original chiral center.

Significance of the Reaction and Product

Understanding this reaction and its major product has broader implications in organic chemistry.

Applications in Organic Synthesis

- The nitrile group is a versatile intermediate that can be transformed into aldehydes, ketones, amines, and carboxylic acids.
- Stereochemical control allows for the synthesis of enantiomerically pure compounds, critical in drug

development.

Chiral Synthesis and Stereochemistry

- The inversion of configuration exemplifies the SN2 mechanism’s stereospecific nature.
- Such reactions are exploited in asymmetric synthesis to produce desired enantiomers.

Environmental and Safety Considerations

- Handling sodium cyanide requires caution due to its toxicity.
- Proper disposal and safety protocols are essential when working with cyanide reagents.

Summary of the Reaction Pathway and Product Formation

Step	Description	Outcome
1	Nucleophilic attack by CN- from the backside	Inversion of configuration at carbon-1
2	Departure of Br-	Formation of (S)-1-cyano-4-methylhexane
3	Final product: stereochemically inverted nitrile	(S)-1-cyano-4-methylhexane

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Conclusion

Treating (R)-1-bromo-4-methylhexane with sodium cyanide predominantly yields (S)-1-cyano-4-methylhexane through an SN2 mechanism characterized by backside attack and stereochemical inversion. This reaction exemplifies the principles of nucleophilic substitution, stereochemistry, and organic synthesis strategies. Recognizing the major product and understanding its formation pathways are essential for designing synthesis routes, especially in pharmaceutical chemistry where enantiomeric purity can influence biological activity.

By mastering such reactions, chemists can manipulate molecular structures with precision, opening avenues for the development of complex, stereochemically defined compounds. The insights gained from this reaction also underscore the importance of stereochemistry in modern organic chemistry and its applications in various industries.

Keywords: SN2 reaction, stereochemistry, (R)-1-bromo-4-methylhexane, sodium cyanide, enantiomer, nitrile, organic synthesis, chiral center, inversion, nucleophilic substitution

Frequently Asked Questions

What is the major product formed when (R)-1-bromo-4-methylhexane reacts with sodium cyanide?

The major product is (R)-4-methylhexanenitrile, resulting from nucleophilic substitution of bromine by cyanide at C-1.

Does the stereochemistry of (R)-1-bromo-4-methylhexane affect the product formed with sodium cyanide?

Yes, the stereochemistry influences the configuration of the resulting nitrile, but in SN2 reactions like this, the configuration at the chiral center is inverted at the site of substitution.

Is the reaction between (R)-1-bromo-4-methylhexane and sodium cyanide an SN1 or SN2 mechanism?

It proceeds via an SN2 mechanism, which involves a backside attack leading to inversion of configuration at the chiral center.

What type of reaction occurs when sodium cyanide reacts with (R)-1-bromo-4-methylhexane?

It's a nucleophilic substitution reaction, specifically an SN2 reaction, replacing the bromine atom with a cyanide group.

What is the stereochemical outcome at the chiral center after the reaction?

The stereochemistry at the chiral center is inverted, so the product will have the (S) configuration at that position if starting from the (R)-enantiomer.

Can the reaction be used to synthesize chiral nitriles from chiral alkyl halides?

Yes, SN2 reactions with sodium cyanide can produce chiral nitriles, but the stereochemical inversion must be considered in the synthesis.

Are there any notable reaction conditions for this substitution to occur efficiently?

Typically, polar aprotic solvents like DMSO or acetone are used, along with heat, to facilitate the SN2 reaction with sodium cyanide.

What potential side reactions or issues should be considered in this reaction?

Potential side reactions include elimination reactions leading to alkenes, or competing SN1 pathways if the substrate is prone to carbocation formation, though SN2 is favored here.

How does the methyl group at the 4-position influence the reactivity of (R)-1-bromo-4-methylhexane?

The methyl group is an electron-donating substituent that can slightly influence the reactivity by providing steric hindrance or electronic effects, but primary alkyl bromides generally undergo SN2 reactions readily.

Additional Resources

Major Product Formed Upon Treatment Of (R)-1-Bromo-4-methylhexane With Sodium Cyanide: An In-Depth Analysis

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Introduction

Understanding the transformation of organic halides with nucleophiles is fundamental in organic synthesis. When an alkyl halide reacts with sodium cyanide (NaCN), the primary outcome is typically a

nucleophilic substitution that introduces a nitrile group into the molecule. In this detailed review, we will explore the specific case of (R)-1-bromo-4-methylhexane reacting with sodium cyanide, analyze the reaction mechanism, predict the major product, and discuss the stereochemical and synthetic implications of this transformation.

Structural Overview of (R)-1-Bromo-4-methylhexane

Before diving into the reaction details, it is essential to understand the structure of the starting compound:

- Molecular structure: 1-bromo-4-methylhexane
- Chirality: The (R) designation indicates the stereochemistry at the chiral center (if present).
- Functional groups: Alkyl bromide (–Br) attached to the first carbon of a hexane chain.
- Substituents:
- Methyl group at carbon 4.
- Bromine atom at carbon 1.

Structural formula:

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CH3–CHBr–CH2–CH(CH3)–CH2–CH3
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With the stereochemistry specified at the relevant chiral center, the compound exists in the (R)-configuration at the chiral center, which can influence the stereochemical outcome of nucleophilic substitution, especially under certain conditions.

Reaction Context: Nucleophilic Substitution with Sodium Cyanide

Sodium cyanide (NaCN) is a potent nucleophile that provides the cyanide ion (CN−). When reacting with alkyl halides, the typical pathway involves nucleophilic substitution, either via SN2 or SN1 mechanisms, depending on the substrate's nature.

Key considerations:

- Type of alkyl halide: Primary alkyl halides (like the one in question) favor SN2 mechanisms.
- Reaction conditions: Usually require polar aprotic solvents (e.g., DMSO, acetone) to facilitate SN2.
- Stereochemistry: SN2 reactions result in inversion of configuration at the chiral center.

Mechanism of Nucleophilic Substitution with Sodium Cyanide

SN2 mechanism overview:

- The cyanide ion acts as a nucleophile, attacking the electrophilic carbon atom bearing the leaving group (bromine).
- The attack occurs from the backside, leading to a one-step concerted process.
- The leaving group (bromide ion, Br−) departs simultaneously with the nucleophile's attack.

Step-by-step process:

1. Nucleophile approaches: The cyanide ion approaches the electrophilic carbon from the side opposite to the bromine atom.
2. Transition state formation: A pentavalent transition state forms, with partial bonds to both the departing bromide and incoming cyanide.
3. Departure of bromide: The bromide leaves, completing the substitution.
4. Product formation: The resulting molecule has a nitrile group attached where the bromine was, and

the stereochemistry at the chiral center is inverted (if applicable).

Predicting the Major Product

Given that (R)-1-bromo-4-methylhexane undergoes SN2 substitution:

- Primary alkyl halide: The reaction predominantly proceeds via SN2.
- Stereochemical implications: The configuration at the chiral center is inverted during SN2. If the original molecule is (R), then the product will be (S) at that specific chiral center.

Major product:

- Structural formula:

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CH3–CH(CN)–CH2–CH(CH3)–CH2–CH3
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- Name: (S)-1-Cyano-4-methylhexane

Key points:

- The bromine atom at carbon 1 is replaced by a nitrile group (–CN).
- The stereochemistry is inverted, transforming the (R)-configuration into (S).

Stereochemical Considerations

- SN2 stereochemistry: The reaction involves backside attack, leading to stereoinversion.
- Chiral center behavior: Since the original (R)-configuration at carbon 1 is inverted, the product's configuration at that center becomes (S).
- Implication for synthesis: This stereochemical change is crucial when the molecule's chiral properties are significant for biological activity or further synthetic steps.

Factors Influencing the Reaction

Several factors impact the efficiency and outcome of this nucleophilic substitution:

- Substrate nature: Primary alkyl halides favor SN2, making the reaction straightforward.
- Solvent choice: Polar aprotic solvents (DMSO, DMF, acetone) enhance nucleophilicity of CN^-.
- Temperature: Elevated temperatures can increase reaction rates but may favor competing elimination (though less likely with primary halides).
- Steric hindrance: The methyl group at carbon 4 does not significantly hinder nucleophilic attack at carbon 1.

Alternative Pathways and Side Reactions

While SN2 is predominant here, potential competing processes include:

- SN1 mechanism: Less likely due to primary halide but possible under certain conditions involving polar protic solvents and heat.
- Elimination reactions (E2): Usually minimal with primary halides unless strongly basic conditions or high temperatures are applied.
- Radical pathways: Not typical in this setting.

Synthetic Implications of the Product

The nitrile group introduced through this reaction serves as a versatile synthetic handle:

- Hydrolysis to amines: Nitriles can be converted into primary amines via acid or base hydrolysis.
- Reduction to aldehydes or amines: Catalytic hydrogenation can produce corresponding amines.
- Further functionalization: The nitrile can undergo various transformations, enabling complex molecule synthesis.

Applications:

- Synthesis of pharmaceuticals, agrochemicals, or intermediates.
- Construction of chiral molecules, especially if stereochemical control is maintained.

Summary of Key Points

Aspect	Details
Starting compound	(R)-1-bromo-4-methylhexane
Reagent	Sodium cyanide (NaCN)
Reaction type	Nucleophilic substitution (SN2)
Major product	(S)-1-cyano-4-methylhexane
Mechanism	Backside attack leading to stereoinversion
Stereochemistry	Inversion at the chiral center (R → S)
Reaction conditions	Polar aprotic solvent, moderate temperature
Synthetic utility	Nitrile as a versatile intermediate

Final Remarks

The transformation of (R)-1-bromo-4-methylhexane with sodium cyanide exemplifies a classic SN2 reaction pathway where primary alkyl halides undergo efficient nucleophilic substitution. The key features include the predictable inversion of stereochemistry and formation of a nitrile, which is highly valuable in further synthetic manipulations. Recognizing these mechanistic and stereochemical principles is essential for designing complex synthetic routes and understanding the behavior of chiral alkyl halides in organic chemistry.

References for Further Reading

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In conclusion, the major product formed upon treatment of (R)-1-bromo-4-methylhexane with sodium cyanide is (S)-1-cyano-4-methylhexane, resulting from an SN2 nucleophilic substitution that causes inversion of configuration at the chiral center. This transformation highlights fundamental principles of stereochemistry, nucleophilic substitution mechanisms, and synthetic utility of nitrile intermediates in organic synthesis.

What Is The Major Product Formed Upon Treatment Of R 1

Bromo 4 Methylhexane With Sodium Cyanide

What Is The Major Product Formed Upon Treatment Of R 1 Bromo 4 Methylhexane With Sodium Cyanide

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