Select The Best Reaction Sequence To Make The Following Ketone. CH_3CCH_2CH_2CH_2CH_2CH_3 Propane, NaNH_2

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Understanding how to synthesize specific ketones is a fundamental skill in organic chemistry, especially when designing pathways for complex molecule construction. In this article, we will explore the optimal reaction sequence to produce the ketone with the structure CH_3CCH_2CH_2CH_2CH_2CH_3, using sodium amide (NaNH_2) as a key reagent. We will analyze the starting materials, potential intermediates, and the step-by-step reactions necessary to achieve this goal efficiently and selectively.

Understanding the Target Molecule and Reagent

Before diving into the synthesis pathway, it is essential to comprehend the structure of the target ketone and the role of NaNH_2 in organic reactions.

Structure of the Target Ketone

The molecular formula is CH_3CCH_2CH_2CH_2CH_2CH_3, which can be interpreted as a six-carbon chain with a ketone functional group. The placement indicates a ketone at the second carbon, making it a 2-hexanone.

- Key features:
- Six carbon atoms in total.
- Ketone functional group at C-2.
- Alkyl chain extending from the ketone.

Role of NaNH_2 in Organic Synthesis

Sodium amide (NaNH_2) is a strong, non-nucleophilic base. Its primary functions include:

- Generating acetylide ions from terminal alkynes.
- Facilitating elimination reactions.
- Acting as a base to deprotonate acidic hydrogens.

In synthesis pathways, NaNH_2 is often used to produce acetylide ions, which serve as nucleophiles in carbon-carbon bond-forming reactions such as nucleophilic acyl substitutions or alkylations.

Strategic Planning for the Synthesis

Creating the target ketone from simpler starting materials requires a well-thought-out sequence. The main considerations include:

- Choosing appropriate starting materials.
- Identifying key reactions (e.g., alkylation, acylation, oxidation).
- Ensuring selectivity and avoiding side reactions.

Given the starting reagent $NaNH_2$, a logical approach involves generating a nucleophilic acetylide intermediate and then performing chain extension reactions to reach the desired six-carbon ketone.

Potential Starting Materials

- Terminal Alkynes: e.g., acetylene ($HC\equiv CH$) or methyl acetylene (propyne).
- Alkyl Halides: e.g., methyl iodide, ethyl bromide, etc.
- Carbonyl Compounds: e.g., acyl chlorides or esters, for ketone formation.

Reaction Pathways Overview

1. Formation of Acetylide Ion: Deprotonate a terminal alkyne with $NaNH_2$.
2. Alkylation of Acetylide: Attach a suitable alkyl group to extend the carbon chain.
3. Oxidation or Carbonyl Introduction: Convert the terminal alkyne or alkylated intermediate into a ketone.

This sequence allows for precise control over chain length and functional group placement.

Step-by-Step Reaction Sequence

Below is a detailed pathway for synthesizing the target ketone.

Step 1: Generation of the Acetylide Ion

- Reactant: Acetylene ($HC\equiv CH$)
- Reaction:

$HC\equiv CH + NaNH_2 \rightarrow HC\equiv C^- Na^+ + NH_3$

- Outcome: Formation of a nucleophilic acetylide ion.

Step 2: Alkylation of the Acetylide Ion

- Reactant: Alkyl halide (e.g., methyl iodide, CH_3I)
- Reaction:

$HC\equiv C^- + CH_3I \rightarrow CH_3-C\equiv C^- + I^-$

Note: The acetylide ion reacts with methyl iodide to form propyne (methyl acetylene).

- Result: Methyl acetylene ($CH_3-C\equiv CH$), which can be further manipulated.

Step 3: Chain Extension via Alkylation

- To extend the chain further to six carbons, use a longer alkyl halide such

as 1-bromopentane ($C_5H_{11}Br$):

$HC\equiv C^- + C_5H_{11}Br \rightarrow C_5H_{11}-C\equiv C^- + Br^-$

- Outcome: Formation of a pentynyl acetylide intermediate, which upon protonation will give 1-pentyne.

Step 4: Conversion of Alkynes to Ketones

- Method: Partial hydrogenation followed by oxidation or direct hydrolysis can convert terminal alkynes into ketones.

- Alternative approach: Use of acyl chlorides with acetylide ions to directly form β-diketones, which can be dehydrated to form enones or ketones.

- Specific reaction:

$C_5H_{11}-C\equiv C^-$ + acyl chloride (e.g., acetyl chloride) → β-ketoester or β-diketone.

- Subsequent oxidation: Use of oxidizing agents (e.g., PCC, Jones reagent) to convert the intermediate into the desired ketone.

Step 5: Final Ketone Formation

- From the extended chain with a terminal alkyne, perform hydrolysis or oxidation to produce the target 2-hexanone:

$CH_3-CH_2-CH_2-CH_2-C(=O)-CH_3$

- Confirming the structure: The final product aligns with the target ketone structure, with the carbonyl at the second position.

Alternative Synthetic Strategies

While the above sequence leverages acetylide chemistry, alternative methods can include:

Using Grignard Reagents and Acyl Chlorides

- Prepare a Grignard reagent (e.g., methyl magnesium bromide).
- React with an acyl chloride (butanoyl chloride) to produce a ketone directly.

Oxidation of Secondary Alcohols

- Synthesize a secondary alcohol with the correct carbon skeleton.
- Oxidize using PCC or Jones reagent to yield the ketone.

Optimizing the Reaction Sequence for Efficiency

To ensure the best results, consider these tips:

- Use pure, anhydrous reagents to prevent side reactions.
- Control reaction temperatures carefully.
- Monitor reactions with TLC or GC-MS.
- Purify intermediates via distillation or chromatography.

Conclusion: The Best Reaction Sequence

In summary, the most efficient route to synthesize the target ketone $CH_3CCH_2CH_2CH_2CH_2CH_3$ utilizing $NaNH_2$ involves:

1. Generating acetylide ions from terminal alkynes with $NaNH_2$.
2. Alkylating acetylide ions with appropriate alkyl halides to extend the

carbon chain.
3. Converting the extended alkyne intermediates into ketones via oxidation or acylation.
4. Final oxidation or hydrolysis steps to produce the desired 2-hexanone.

This pathway leverages the power of acetylide chemistry to achieve selective chain extension and functional group transformation, ensuring the synthesis is both efficient and high-yielding.

Keywords: organic synthesis, ketone synthesis, reaction sequence, NaNH_2, acetylide, chain extension, alkylation, oxidation, 2-hexanone, acetylene, alkyl halides

Frequently Asked Questions

What is the main goal when selecting a reaction sequence to synthesize a ketone from propane using $NaNH_2$?

The goal is to introduce a carbonyl group at the appropriate position by converting a suitable precursor through steps like deprotonation and subsequent reactions, ultimately leading to the desired ketone.

Why is $NaNH_2$ used in the reaction sequence to synthesize the ketone from propane?

$NaNH_2$ is a strong base used to generate a carbanion or deprotonate terminal alkynes, facilitating nucleophilic addition or substitution reactions necessary to form the ketone.

Which intermediate is typically formed when using $NaNH_2$ in the synthesis of a ketone from a hydrocarbon?

A terminal alkyne or a carbanion intermediate is formed, which then undergoes

further reactions such as nucleophilic attack on suitable electrophiles to form the desired ketone.

What is the significance of the chain length in the starting hydrocarbon, such as propane, for forming the ketone?

The chain length determines the position of the carbonyl group in the final ketone, ensuring proper placement for the desired structure after the reaction sequence.

Which reagent is typically used after $NaNH_2$ to convert the intermediate into the ketone?

Usually, an electrophile like methyl iodide or other alkyl halides is used to alkylate the carbanion intermediate, followed by oxidation or hydrolysis steps to form the ketone.

Is it necessary to perform a halogenation step before forming the ketone from propane? Why or why not?

Yes, halogenation (e.g., bromination) can be necessary to introduce a good leaving group, which can then be displaced by nucleophiles during the synthesis of the ketone.

What is the overall sequence of reactions to convert propane into the specified ketone using $NaNH_2$?

The sequence typically involves halogenation to form a halide, deprotonation with $NaNH_2$ to generate a carbanion, nucleophilic substitution with suitable electrophiles, and oxidation or hydrolysis to yield the ketone.

What are the key considerations when designing a reaction sequence to synthesize a ketone from a simple hydrocarbon like propane?

Key considerations include selecting appropriate halogenation steps, controlling reaction conditions to favor desired intermediates, and ensuring proper functional group transformations to introduce the carbonyl group at the correct position.

Can you directly convert propane into the target ketone using $NaNH_2$ alone? Why or why not?

No, $NaNH_2$ alone cannot directly convert propane into the ketone; it requires a multi-step sequence involving halogenation, formation of reactive intermediates, and subsequent reactions to achieve the final product.

Additional Resources

Select The Best Reaction Sequence To Make The Following Ketone: $CH_3C(CH_2)_5CH_3$ from Propane, $NaNH_2$

In the realm of organic synthesis, transforming simple hydrocarbons into more complex functionalized molecules is a fundamental challenge that demands a deep understanding of reaction mechanisms, reagent behaviors, and strategic planning. The particular task of synthesizing a ketone such as $CH_3C(CH_2)_5CH_3$—a methyl-substituted hexanone—starting from propane and employing sodium amide ($NaNH_2$) exemplifies this complexity. This article aims to analyze and delineate the most effective sequence of reactions to achieve this transformation, emphasizing the strategic considerations that underpin successful synthesis pathways.

Understanding the Target Molecule and Starting Material

The Target Ketone: Structural and Functional Aspects

The target molecule, $CH_3C(CH_2)_5CH_3$, is a six-carbon ketone with the carbonyl group (C=O) positioned at the second carbon in the chain, flanked by methyl groups. Its systematic name is 2-hexanone. The structure can be visualized as:

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CH3-C(=O)-(CH2)4-CH3
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This molecule features a carbonyl group at C-2, with a total chain length of six carbons, making it a straightforward member of the ketone family. The presence of the carbonyl group allows for various nucleophilic additions and further functionalizations, but the challenge lies in constructing this skeleton from simple hydrocarbons.

The Starting Material: Propane

Propane ($CH_3-CH_2-CH_3$) is an alkane with three carbons, characterized by high stability and low reactivity due to its saturated nature. The task involves extending the carbon chain and introducing the carbonyl functionality at the appropriate position, which requires strategic carbon–carbon bond formation and functional group transformations.

Role of $NaNH_2$ in Organic Synthesis

$NaNH_2$ (sodium amide) is a strong, non-nucleophilic base commonly used in organic synthesis to generate carbanions via deprotonation of terminal

alkynes or other acidic hydrogens. Its primary utility in chain-extension and functional group transformations involves:

- Generating acetylide ions from terminal alkynes
- Facilitating nucleophilic addition to electrophiles
- Enabling carbon–carbon bond formation through nucleophilic attack

In this context, $NaNH_2$ is likely to be used to generate a reactive nucleophile (such as an acetylide ion) that can attack an electrophilic carbon to extend the chain, ultimately leading to the formation of the desired ketone.

Strategic Approach to the Synthesis

The overarching goal is to construct the six-carbon chain with the correct placement of the carbonyl group. A logical strategy involves:

1. Chain Extension: Using acetylide chemistry to add carbons to propane
2. Functionalization: Introducing the carbonyl group at the correct position
3. Oxidation or Oxidative Workup: Converting suitable intermediates into ketones

The key is to leverage the reactivity of alkynes generated by $NaNH_2$ to perform nucleophilic additions that extend the carbon chain, followed by oxidation to form the ketone.

Proposed Reaction Sequence

Based on the analysis, a viable sequence involves:

Step 1: Formation of Acetylide Ion from Terminal Alkyne

- React propane with a suitable terminal alkyne precursor, such as acetylene (ethyne), in the presence of $NaNH_2$.
- $NaNH_2$ deprotonates acetylene to generate the acetylide ion ($-C\equiv C^-$), a potent nucleophile capable of adding to electrophiles.

Step 2: Chain Extension via Nucleophilic Attack

- The acetylide ion reacts with a suitable electrophile, such as methyl iodide (CH_3I) or ethyl iodide (C_2H_5I), to extend the chain by one or more carbons.
- For example, attacking methyl iodide yields propyne ($HC\equiv C-CH_3$), a linear alkyne with four carbons.

Step 3: Building the Correct Chain Length

- Repeat the deprotonation and alkylation steps to reach the desired chain length of six carbons.
- For instance, sequentially adding methyl groups to extend from propane to hex-4-yne.

Step 4: Conversion of Alkynes to Ketones

- Use alkyne hydration (Markovnikov or anti-Markovnikov addition) to convert the terminal or internal alkyne into a ketone.
- Catalysts such as mercuric ion (Hg^{2+}) or acidic conditions facilitate this hydration, leading to the formation of a ketone.

Step 5: Oxidation and Final Functionalization

- The resulting enol or enolate intermediates tautomerize to ketones.
- Final oxidation steps ensure the correct placement of the carbonyl group at the second carbon, producing 2-hexanone.

Detailed Reaction Pathway and Rationale

1. Generation of Acetylide from Terminal Alkyne

- React acetylene ($HC\equiv CH$) with $NaNH_2$ in liquid ammonia or another aprotic solvent.
- Equation:

$$HC\equiv CH + NaNH_2 \rightarrow Na^+ -C\equiv C^- + NH_3$$

- The acetylide ion is a strong nucleophile, ready for subsequent alkylation.

2. Chain Extension via Alkylation

- Alkylate the acetylide with methyl iodide (or ethyl iodide) to extend the carbon chain:

$$Na^+ -C\equiv C^- + CH_3I \rightarrow HC\equiv C-CH_3 + NaI$$

- Repeating this process enables the construction of longer carbon chains, moving from propane toward hexane.

3. Hydration of Internal or Terminal Alkynes

- Once the desired chain length is reached, perform alkyne hydration:

$$HC\equiv C-(CH_2)_3-CH_3 + Hg^{2+}/H_2SO_4 \rightarrow CH_3-C(=O)-(CH_2)_4-CH_3 \text{ (a ketone)}$$

- This step converts the alkyne to a methyl ketone, with the carbonyl at the appropriate position.

4. Selective Oxidation and Tautomerization

- The enol form tautomerizes into the ketone, giving the target molecule $CH_3C(CH_2)_5CH_3$.

Alternative Strategies and Considerations

While the above approach leverages familiar reaction mechanisms, alternative pathways exist:

- Alkylation of Acetylide followed by Oxidative Cleavage:
Constructing a longer chain first, then cleaving or modifying as needed.

- Use of Grignard Reagents:
Forming Grignard reagents from halogenated precursors, then adding to carbonyl compounds.

- Sequential Functionalizations:
Starting from simpler molecules like acetaldehyde or acetic acid derivatives to install the carbonyl directly.

However, given the starting point (propane) and the reagents ($NaNH_2$), the acetylide chemistry route remains the most straightforward and effective.

Summary and Conclusion

Transforming propane into $CH_3C(CH_2)_5CH_3$ via a reaction sequence involving $NaNH_2$ demands a strategic approach centered on chain extension and functional group transformations. The most effective pathway involves:

- Generating acetylide ions from terminal alkynes using $NaNH_2$
- Performing sequential alkylations to build the six-carbon chain
- Hydrating the alkyne to form the methyl ketone

- Ensuring regioselectivity and proper positioning of the carbonyl group through controlled hydration and oxidation

This sequence leverages the strong base properties of $NaNH_2$, the nucleophilicity of acetylide ions, and the well-understood hydration chemistry of alkynes to achieve the target ketone efficiently. Such a pathway underscores the importance of fundamental organic reactions—nucleophilic addition, alkylation, hydration, and oxidation—in complex molecule synthesis.

In conclusion, the best reaction sequence involves:

1. Deprotonation of acetylene with $NaNH_2$ to generate acetylide ions.
2. Sequential alkylation with methyl iodide to extend the carbon chain to six carbons.
3. Hydration of the internal alkyne to form the ketone at the correct position.
4. Final tautomerization and oxidation to yield the desired 2-hexanone.

This strategic synthesis pathway exemplifies the power of classical organic chemistry tools and reaction mechanisms in constructing complex molecules from simple hydrocarbons.

Select The Best Reaction Sequence To Make The Following Ketone Ch 3cch 2ch 2ch 2ch 3 Propane Nanh 2

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