Give The Structure Of The Principal Organic Product Formed By Free-radical Bromination Of 2,2,4trimethylpentane.

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Understanding the principles of free radical substitution reactions, particularly bromination, is fundamental in organic chemistry. When a hydrocarbon like 2,2,4-trimethylpentane undergoes free radical bromination, the reaction predominantly yields a specific mono-brominated product. This product's structure is determined by the stability of the free radicals formed during the process and the accessibility of various hydrogen atoms within the molecule. In this article, we will explore the detailed mechanism of free-radical bromination, analyze the structure of 2,2,4-trimethylpentane, identify the most reactive sites, and ultimately determine the principal organic product formed.

Introduction to Free Radical Bromination

Free radical bromination is a substitution reaction where a bromine atom replaces a hydrogen atom on an organic molecule via a radical chain mechanism. This reaction is initiated by a radical initiator (such as a peroxide or light), propagates through a series of radical steps, and terminates when radicals combine.

Key features of free radical bromination:
- It predominantly produces mono-brominated products.
- The selectivity is influenced by the stability of the intermediate radicals.
- Bromination tends to occur at the most reactive (most stable) hydrogen sites in the molecule.

Overview of 2,2,4-Trimethylpentane

Before analyzing the bromination product, it is essential to understand the structure of 2,2,4-trimethylpentane.

Structural Formula and Configuration

2,2,4-Trimethylpentane, also known as isoheptane, has the molecular formula C8H18. Its structural formula can be described as:

```
CH3
|
CH3-CH-CH2-CH-CH3
| |
CH3 CH3
```

In a more detailed linear perspective:

- The main chain is a pentane chain (5 carbons).
- At carbon 2 (second carbon from the end), two methyl groups are attached.
- At carbon 4, one methyl group is attached.

Structural features:
- The molecule is highly branched.
- The branching at carbons 2 and 4 creates tertiary and secondary carbons.
- The presence of methyl groups affects the reactivity of hydrogen atoms due to their environment.

Numbering the Carbon Chain

Numbering the chain from one end (say, the left):

1. Carbon 1 (end of the chain)
2. Carbon 2 (bearing two methyl groups)
3. Carbon 3
4. Carbon 4 (bearing one methyl group)
5. Carbon 5 (end of the chain)

The methyl groups are attached at carbons 2 and 4, which are key sites for radical formation during bromination.

Identification of Reactivity Sites in 2,2,4-Trimethylpentane

The selectivity of free radical bromination depends largely on the stability of the resulting radical intermediates, which in turn depends on the type of

carbon (primary, secondary, tertiary).

Types of carbons in 2,2,4-trimethylpentane:

- Primary carbons: attached to only one other carbon.
- Secondary carbons: attached to two other carbons.
- Tertiary carbons: attached to three other carbons.

Distribution of hydrogen atoms:

Carbon Type	Number of Hydrogens	Number of Carbons	Relative Reactivity
Primary	Several (on terminal methyls)	5	Least reactive
Secondary	On the main chain, not adjacent to methyl groups	Moderate	More reactive than primary
Tertiary	At carbons 2 and 4 (where methyl groups are attached)	Fewer hydrogens but more reactive	Most reactive sites

Key insight:
Hydrogens attached to tertiary carbons are most susceptible to abstraction because radicals formed here are more stable (due to greater alkyl substitution stabilizing the radical via hyperconjugation and inductive effects).

Radical Stability and Site Selectivity

Radical stability follows the order:

Tertiary > Secondary > Primary

In 2,2,4-trimethylpentane:

- The tertiary carbons at C-2 and C-4 are the most reactive sites.
- Hydrogen abstraction from these tertiary carbons leads to the most stable radical intermediates.

Implication:

Bromination will predominantly occur at the tertiary carbons C-2 and C-4, leading to the formation of mono-brominated products at these sites.

Mechanism of Free-Radical Bromination of 2,2,4-Trimethylpentane

The bromination proceeds via a radical chain mechanism consisting of three main steps:

1. Initiation

- Homolytic cleavage of Br2 molecule under light or heat generates two bromine radicals:

$$
\mathrm{Br}_2 \xrightarrow{hv \text{ or heat}} 2 \mathrm{Br}^\bullet
$$

2. Propagation

- Hydrogen abstraction:

$$
\mathrm{Br}^\bullet + \mathrm{RH} \rightarrow \mathrm{HBr} + \mathrm{R}^\bullet
$$

- Radical recombination:

$$
\mathrm{R}^\bullet + \mathrm{Br}_2 \rightarrow \mathrm{RBr} + \mathrm{Br}^\bullet
$$

- The most probable hydrogen abstraction occurs at tertiary carbons due to radical stability.

3. Termination

- Two radicals combine to terminate the chain:

$$
\mathrm{R}^\bullet + \mathrm{R'}^\bullet \rightarrow \mathrm{RR'}
$$

Principal Organic Product of Bromination

Given the stability considerations and reactivity pattern, the dominant product will be the mono-brominated compound formed by substitution at the most reactive (tertiary) sites.

Expected major products:

- Bromination at C-2 (tertiary carbon attached to two methyl groups)
- Bromination at C-4 (another tertiary carbon with a methyl group attached)

Because both C-2 and C-4 are tertiary and equally reactive, the reaction may yield a mixture of two mono-brominated isomers.

Structure of the Principal Organic Product

The principal product will be 2-bromo-2,4-trimethylpentane or 4-bromo-2,4-trimethylpentane, depending on which tertiary carbon is brominated.

Structural description:

- The bromine atom replaces one hydrogen at either C-2 or C-4.
- The rest of the molecule remains unchanged.
- The product retains the same primary and secondary carbons, with only the substitution at the tertiary position.

Example:

- Bromination at C-2:

```
CH3
|
CH3-CH-CH2-CH-CH3
| |
CH3 CH3
```

becomes

```
CH3
|
CH3-CH(Br)-CH2-CH-CH3
| |
CH3 CH3
```

```

Similarly, at C-4:

```
CH3
|
CH3-CH-CH2-CH(Br)-CH3
| |
CH3 CH3
```

---

## Summary and Key Takeaways

- The free radical bromination of 2,2,4-trimethylpentane predominantly targets tertiary hydrogens due to radical stability.
- The major products are mono-brominated compounds at either C-2 or C-4.
- Due to symmetry and similar reactivity, both mono-brominated isomers are formed in approximately equal amounts.
- The principal organic product is thus a mixture of 2-bromo-2,4-trimethylpentane and 4-bromo-2,4-trimethylpentane.

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## Conclusion

In conclusion, the structure of the principal organic product formed by free-radical bromination of 2,2,4-trimethylpentane is a mono-brominated derivative at the most reactive tertiary carbons, specifically at carbons 2 and 4. The dominant products are 2-bromo-2,4-trimethylpentane and 4-bromo-2,4-trimethylpentane, formed via radical abstraction at the tertiary sites, which are stabilized by hyperconjugation and inductive effects. Understanding this selectivity is crucial for predicting the outcomes of radical halogenation reactions in complex hydrocarbons, facilitating targeted synthesis and functionalization in organic chemistry.

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Frequently Asked Questions

What is the principal organic product formed by free-radical bromination of 2,2,4-trimethylpentane?

The principal product is 2-bromo-2,4-trimethylpentane, where bromination occurs at the most stable tertiary carbon center.

Why does free-radical bromination of 2,2,4-trimethylpentane favor substitution at a particular carbon atom?

Because free radicals favor forming at the most stable radical site, which in this case is the tertiary carbon at C-2, leading to bromination at that position.

Which carbon position in 2,2,4-trimethylpentane is most susceptible to bromination under free-radical conditions?

The tertiary carbon at the 2-position is most susceptible due to the stability of the tertiary radical intermediate formed during the reaction.

What is the significance of the stability of radical intermediates in determining the product of free-radical bromination?

More stable radical intermediates lead to higher reaction rates and determine the major product, favoring substitution at the most stable radical site.

How does the structure of 2,2,4-trimethylpentane influence the regioselectivity of bromination?

The presence of multiple methyl groups creates tertiary carbons with greater radical stability, directing bromination to the tertiary position at C-2.

Can you illustrate the structure of the principal

product formed by bromination of 2,2,4-trimethylpentane?

Yes, the principal product is 2-bromo-2,4-trimethylpentane, where bromine attaches at the tertiary carbon at position 2, maintaining the rest of the structure intact.

Additional Resources

Give The Structure Of The Principal Organic Product Formed By Free-radical Bromination Of 2,2,4-trimethylpentane

Understanding the structure of the principal organic product formed by free-radical bromination of 2,2,4-trimethylpentane involves delving into the nuances of free radical chemistry, substitution patterns, and the stability of possible radical intermediates. This topic is a classic example in organic chemistry, illustrating how selective halogenation occurs in complex alkanes and how the stability of radical intermediates guides the regioselectivity of the reaction.

Introduction to Free-Radical Bromination

Free-radical bromination is a fundamental organic reaction used to selectively substitute hydrogen atoms in alkanes with bromine atoms. It proceeds via a radical chain mechanism involving initiation, propagation, and termination steps.

Basic Mechanism Overview

- Initiation: Formation of bromine radicals through homolytic cleavage of Br–Br bonds, usually initiated by heat or light.
- Propagation: Radical attack on the alkane, forming an alkyl radical and hydrogen bromide (HBr). The alkyl radical then reacts with bromine molecules to generate the brominated product and regenerate a bromine radical.
- Termination: Two radicals combine to form stable, neutral molecules, ending the chain process.

In alkanes with multiple hydrogens, the key factor dictating which hydrogen is abstracted is the relative stability of the resulting alkyl radicals.

Structural Features of 2,2,4-Trimethylpentane

Before analyzing the bromination, it is essential to understand the structure of 2,2,4-trimethylpentane:

- The base chain is a pentane backbone: $CH_3–CH_2–CH_2–CH_2–CH_3$.
- There are methyl groups attached at carbons 2 and 4:
- At carbon 2: two methyl groups (making it a 2,2-dimethyl substituent).
- At carbon 4: one methyl group.

This substitution pattern creates a bulky, branched structure with tertiary and secondary hydrogens. The branching influences the radical stability and, consequently, the site of bromination.

Structural Diagram (Simplified)

```
CH₃
|
CH₃–CH–CH₂–CH–CH₃
| |
CH₃ CH₃
```

- The methyl groups at carbons 2 and 4 create quaternary, tertiary, and secondary carbons, affecting where the bromination is most favorable.

Radical Stability and Site Selectivity

Radical Stability Hierarchy

The relative stability of alkyl radicals influences where bromination occurs:

- Tertiary radicals > Secondary radicals > Primary radicals

The stability difference arises because tertiary radicals are stabilized by hyperconjugation and inductive effects from neighboring alkyl groups.

Implication in Bromination

Given the structure of 2,2,4-trimethylpentane, potential sites for radical formation include:

- Primary hydrogens: attached to primary carbons (least stable radicals).
- Secondary hydrogens: attached to secondary carbons.
- Tertiary hydrogens: attached to tertiary carbons (most stable radicals).

The reaction predominantly occurs at the site where the resulting radical is most stable.

Analyzing Possible Bromination Sites in 2,2,4-Trimethylpentane

Step 1: Identify unique hydrogen environments

- Carbons 1 and 5: terminal methyl groups (primary carbons).
- Carbons 2 and 3: methylene groups (secondary carbons).
- Carbons 4: methyl group attached to a quaternary carbon (but the methyl itself is primary hydrogens).

Step 2: Determine which hydrogens are most reactive

- Hydrogens on tertiary carbons (if any) are most reactive.
- Hydrogens on secondary carbons are less reactive but still significant.
- Hydrogens on primary carbons are least reactive due to lower radical stability.

Step 3: Locate tertiary or secondary carbons

- The carbon at position 2 is bonded to two methyl groups, making it quaternary.
- The carbon at position 4 also bears a methyl substituent but is attached to a secondary carbon backbone, making it tertiary.

Therefore, the most reactive site is likely to be the tertiary hydrogen at the 4th carbon.

Determining the Principal Product

The Role of Tertiary Hydrogen Abstraction

During free-radical bromination, abstraction of tertiary hydrogens is favored due to the stability of the resulting tertiary radical. Consequently, the major brominated product will be formed by substitution at the tertiary carbon with the most accessible tertiary hydrogen.

Step-by-Step Prediction of the Product

1. Identify the most reactive hydrogen

- The tertiary hydrogen at carbon 4 is most prone to abstraction.
- Bromination at this site yields a tertiary radical intermediate.

2. Radical formation

- Bromine radical abstracts a hydrogen from the tertiary carbon at position 4.
- The resulting radical is stabilized by the surrounding methyl groups.

3. Radical bromination yields the principal product

- The radical intermediate reacts with a bromine molecule (Br_2) to give the brominated compound.

4. Final structure of the principal product

- Bromine replaces a hydrogen at carbon 4, which is attached to a methyl group.

Structure of the Principal Organic Product

The principal product is 4-bromo-2,2,4-trimethylpentane.

Structural features:

- The bromine atom is attached to the tertiary carbon at position 4.
- The rest of the structure remains unchanged.

Visual Representation

```
CH₃
|
CH₃–C–CH₂–C–CH₃
| |
CH₃ CH₂Br
```

- The bromine is attached to the carbon at position 4, which is tertiary.

Additional Considerations

Regioselectivity and Reaction Conditions

- Free-radical bromination tends to be less selective than chlorination, but the regioselectivity still favors more stable radical sites.
- Reaction conditions, such as light or heat, influence radical initiation and overall reaction efficiency.
- Steric hindrance can also influence the site of bromination, especially in such branched molecules.

Possible Minor Products

- Bromination at secondary carbons (less stable radicals) can occur but will be in minor amounts.
- Primary hydrogens are least reactive and contribute negligibly to the

product mixture.

Summary and Key Takeaways

- The principal organic product from free-radical bromination of 2,2,4-trimethylpentane is 4-bromo-2,2,4-trimethylpentane.
- The site of substitution is the tertiary hydrogen at carbon 4, owing to the higher stability of the tertiary radical intermediate.
- Understanding radical stability, steric effects, and the structure of the substrate is essential for predicting regioselectivity.

Final Thoughts

The analysis of free-radical halogenation reactions demonstrates the importance of radical stability and molecular structure in determining reaction pathways and products. In branched alkanes like 2,2,4-trimethylpentane, the reaction's regioselectivity underscores the influence of tertiary and secondary radical stability, guiding chemists in predicting and controlling halogenation outcomes. Mastery of these principles is fundamental in organic synthesis, enabling the design of selective halogenation strategies for complex molecules.

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