Give The IUPAC Name For The Following Compound: Multiple Choice (1R,3R)-1-ethyl-3-methylcyclohexane (1S,3S)-1-ethyl-3-methylcyclohexane

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Understanding the IUPAC Nomenclature and Stereochemistry of Cyclohexane Derivatives

The process of naming organic compounds systematically is governed by the International Union of Pure and Applied Chemistry (IUPAC) nomenclature rules. When dealing with cyclohexane derivatives, especially those with multiple substituents and stereochemistry, the nomenclature becomes more intricate. In this article, we will explore the principles involved in naming compounds such as (1R,3R)-1-ethyl-3-methylcyclohexane and (1S,3S)-1-ethyl-3-methylcyclohexane, emphasizing the importance of stereochemistry and substituent prioritization.

Introduction to Cyclohexane and Its Substituted Derivatives

Cyclohexane is a cyclic hydrocarbon with the molecular formula C_6H_{12}. Its conformational flexibility allows for various substituents to attach at different positions, resulting in numerous stereoisomers. When substituents are attached to cyclohexane, they can be oriented in axial or equatorial positions, which influences the compound's stability and reactivity.

Key points:

- The numbering of the cyclohexane ring starts at the substituent that provides the lowest possible numbers.
- Substituents are prioritized based on the Cahn-Ingold-Prelog (CIP) rules when assigning stereochemistry.
- Stereoisomers are distinguished as enantiomers or diastereomers, based on the configuration at chiral centers.

Deciphering the Compound Names: (1R,3R)-1-ethyl-3-methylcyclohexane and (1S,3S)-1-ethyl-3-methylcyclohexane

The two compounds in question are stereoisomers, specifically enantiomers, due to the opposite configurations at the chiral centers.

Understanding the notation:

- (1R,3R): Indicates that the substituents at carbons 1 and 3 are in the R configuration.
- (1S,3S): Indicates the opposite stereochemistry at the same positions.

Both compounds have the same substituents: an ethyl group at carbon 1 and a methyl group at carbon 3, but differ in spatial arrangement.

Step-by-Step Approach to Assigning IUPAC Names

To accurately name these compounds, one must understand the process of:

1. Identifying the parent chain: Cyclohexane.
2. Numbering the ring: Assigning the lowest possible numbers to the substituents.
3. Locating substituents: Ethyl and methyl groups at carbons 1 and 3, respectively.
4. Determining stereochemistry: Assigning R or S configurations at each chiral center.
5. Constructing the full name: Combining all elements following IUPAC rules.

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1. Numbering and Substituent Placement

- The ring is numbered to give the lowest possible numbers to the substituents.
- The ethyl group is at carbon 1.
- The methyl group is at carbon 3.

Since both positions are assigned, the numbering is straightforward.

Note: If substituents are on the same side (both R or both S), the stereoisomer is enantiomer; if not, they are diastereomers.

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2. Determining Stereochemistry at Each Chiral Center

- Each chiral center is at carbons 1 and 3.
- The configuration (R or S) is based on the CIP priority rules, considering the substituents attached to each carbon.

Assigning R or S:

- Step 1: Assign priorities to substituents attached to the chiral center.
- Step 2: Orient the molecule so that the lowest priority group is directed away.
- Step 3: Determine the sequence of the groups 1→2→3; clockwise indicates R, counterclockwise indicates S.

Understanding Chirality and Stereoisomerism in Cyclohexane

Cyclohexane derivatives often exhibit stereoisomerism due to the three-dimensional arrangements of substituents. The two key types are:

- Enantiomers: Non-superimposable mirror images (e.g., (1R,3R) vs. (1S,3S))

- Diastereomers: Stereoisomers that are not mirror images (e.g., (1R,3R) vs. (1R,3S))

In our case, (1R,3R) and (1S,3S) are enantiomers, which means they have identical physical properties except for optical activity.

How to Differentiate and Name the Stereoisomers

When naming stereoisomers, the focus is on:

- The configuration at each chiral center.
- The overall relationship between the stereoisomers (enantiomers vs. diastereomers).

For (1R,3R)-1-ethyl-3-methylcyclohexane:

- Both centers have R configuration.
- The compound is a specific stereoisomer with a defined three-dimensional arrangement.

For (1S,3S)-1-ethyl-3-methylcyclohexane:

- Both centers have S configuration.
- It is the enantiomer of the (1R,3R) compound.

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3. Confirming the Correct IUPAC Name

The IUPAC name for these compounds follows the pattern:

- Name of the parent: cyclohexane
- Number and position of substituents: 1-ethyl, 3-methyl
- Stereochemistry: (1R,3R) or (1S,3S)

Complete names:

- (1R,3R)-1-ethyl-3-methylcyclohexane
- (1S,3S)-1-ethyl-3-methylcyclohexane

These names explicitly indicate the stereochemistry and substitution pattern.

Importance of Stereochemistry in Organic Chemistry

Stereochemistry significantly impacts the physical and chemical properties of compounds, including:

- Optical activity
- Biological activity
- Reactivity

Understanding stereochemistry is crucial in fields such as pharmaceuticals, where enantiomers can have

different biological effects.

Common Mistakes and Clarifications

- Confusing R and S configurations: Always verify priorities and orientations.
- Misnumbering: Ensure substituents receive the lowest possible numbers.
- Overlooking stereochemistry: Both configuration and spatial arrangement are essential for accurate naming.

Summary and Final Remarks

In conclusion, the IUPAC names for the given stereoisomers are:

- (1R,3R)-1-ethyl-3-methylcyclohexane
- (1S,3S)-1-ethyl-3-methylcyclohexane

These names precisely describe the position and stereochemistry of the substituents on the cyclohexane ring. Recognizing the difference between enantiomers and diastereomers is vital in organic chemistry, especially when dealing with complex molecules.

Key takeaways:

- Always follow IUPAC rules for numbering and naming.
- Pay careful attention to stereochemistry and CIP priorities.
- Understand the relationship between stereoisomers and their physical properties.

Mastering these principles enables chemists to communicate complex molecular structures clearly and accurately, facilitating advancements in research and industry.

Further Resources

- IUPAC Nomenclature of Organic Chemistry (Blue Book)
- Organic Chemistry Textbooks (e.g., Morrison & Boyd, Solomons)
- Online tools for stereochemistry and naming (e.g., ChemDraw, PubChem)

In summary, correctly naming (1R,3R)-1-ethyl-3-methylcyclohexane and its enantiomer (1S,3S)-1-ethyl-3-methylcyclohexane involves understanding the fundamentals of cyclohexane substitution, stereochemistry, and IUPAC nomenclature rules. Awareness of these concepts enhances clarity in chemical communication and research.

Frequently Asked Questions

What is the IUPAC name for the compound with (1R,3R)-1-ethyl-3-methylcyclohexane?

cis-1-ethyl-3-methylcyclohexane

What is the IUPAC name for the compound with (1S,3S)-1-ethyl-3-methylcyclohexane?

cis-1-ethyl-3-methylcyclohexane

Are the compounds (1R,3R)-1-ethyl-3-methylcyclohexane and (1S,3S)-1-ethyl-3-methylcyclohexane enantiomers or diastereomers?

They are enantiomers.

What stereochemistry do the (1R,3R) and (1S,3S) descriptors indicate about the cyclohexane derivatives?

They indicate opposite configurations at both chiral centers, making them enantiomers.

In the given compounds, what does the 'cis' configuration imply about the substituents on the cyclohexane ring?

It implies that the substituents are on the same face of the cyclohexane ring.

How do you differentiate between (1R,3R) and (1S,3S) stereoisomers in cyclohexane derivatives?

They are stereoisomers with opposite configurations at both chiral centers, representing enantiomers.

Which nomenclature indicates the stereochemistry of the substituents on the cyclohexane ring in these compounds?

The (1R,3R) and (1S,3S) descriptors indicate the stereochemistry.

Can (1R,3R)-1-ethyl-3-methylcyclohexane be considered the mirror image of (1S,3S)-1-ethyl-3-methylcyclohexane?

Yes, they are mirror images and enantiomers.

What is the significance of the 'R' and 'S' labels in the IUPAC naming of these cyclohexane derivatives?

They specify the absolute configuration (spatial arrangement) of the chiral centers.

Are the compounds (1R,3R)- and (1S,3S)-1-ethyl-3-methylcyclohexane optically active?

Yes, both are optically active as enantiomers.

Additional Resources

Understanding the IUPAC Naming of Complex Cyclic Compounds: A Deep Dive into (1R,3R)-1-ethyl-3-methylcyclohexane and (1S,3S)-1-ethyl-3-methylcyclohexane

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Introduction: The Significance of IUPAC Nomenclature in Organic Chemistry

In the realm of organic chemistry, precise communication hinges on a universally accepted nomenclature system. The International Union of Pure and Applied Chemistry (IUPAC) provides such a standardized system, allowing scientists worldwide to accurately identify and discuss chemical compounds. This system becomes particularly crucial when dealing with complex cyclic structures that may have multiple stereoisomers—molecules sharing the same molecular formula but differing in three-dimensional arrangements.

Among these, cyclohexane derivatives bearing various substituents and stereochemistry present an intriguing challenge for chemists. Correctly naming these compounds provides insights into their structure, stereochemistry, and potential reactivity. In this context, understanding the IUPAC names for compounds such as (1R,3R)-1-ethyl-3-methylcyclohexane and (1S,3S)-1-ethyl-3-methylcyclohexane is essential for both academic and practical applications, including synthesis, pharmacology, and material science.

Deciphering the Structural Framework: The Core of Cyclohexane Derivatives

1. The Cyclohexane Ring as a Fundamental Scaffold

Cyclohexane is a six-membered saturated carbocycle exhibiting remarkable conformational flexibility. Its chair conformation is the most stable, minimizing torsional and angle strain. When substituents are attached to this ring, their positions and orientations significantly influence the compound's physical and chemical properties.

2. Substituents: Ethyl and Methyl Groups

In the compounds under discussion, two substituents are attached:

- Ethyl group ($-CH_2CH_3$): A two-carbon alkyl substituent.
- Methyl group ($-CH_3$): A one-carbon alkyl substituent.

Their positions on the cyclohexane ring are numbered to give the lowest possible numbers, following IUPAC rules, and their stereochemistry (R/S configuration) is designated at each chiral center.

Understanding Stereochemistry: R and S Configurations

1. Chirality and Stereocenters

A stereocenter (or chiral center) is a carbon atom bonded to four different substituents, giving rise to stereoisomerism. In cyclic structures like cyclohexane, chiral centers can exist at carbons bearing substituents, especially when substituents are attached in such a way that they create non-superimposable mirror images.

2. R and S Nomenclature

The R/S system describes the absolute configuration around a stereocenter:

- R (Rectus): Latin for "right," indicating a clockwise arrangement of substituents when priorities are assigned.
- S (Sinister): Latin for "left," indicating a counterclockwise arrangement.

The process involves assigning priorities based on atomic numbers, orienting the molecule accordingly, and determining the sequence.

3. Stereoisomerism in the Given Compounds

- (1R,3R)-1-ethyl-3-methylcyclohexane: Both chiral centers at carbons 1 and 3 are in the R configuration.
- (1S,3S)-1-ethyl-3-methylcyclohexane: Both chiral centers at carbons 1 and 3 are in the S configuration.

These stereoisomers are enantiomers—non-superimposable mirror images—each exhibiting distinct spatial arrangements.

Step-by-Step IUPAC Naming Process

1. Identifying the Principal Chain

The principal chain is the cyclohexane ring, which acts as the parent structure. The substituents are attached to this core.

2. Numbering the Ring

- Number the ring to give the substituents the lowest possible numbers.
- Here, both substituents are attached to carbons 1 and 3, which are assigned based on substituents' priorities if necessary.

3. Assigning Substituents and Stereochemistry

- Attach the ethyl and methyl groups to carbons 1 and 3.
- Determine the stereochemistry at each chiral center based on three-dimensional arrangements, leading to R or S designations.

4. Naming the Compound

- Combine the stereochemical descriptors with the substituents and the parent name.
- For example: (1R,3R)-1-ethyl-3-methylcyclohexane.

Distinguishing Between the Enantiomers

The two compounds in question are stereoisomers, specifically enantiomers, which have identical physical properties except for the direction they rotate plane-polarized light and their interactions with other chiral molecules.

- (1R,3R)-1-ethyl-3-methylcyclohexane: Enantiomer with both centers in the R configuration.
- (1S,3S)-1-ethyl-3-methylcyclohexane: The mirror image, with both centers S.

The importance of correctly naming these lies in their stereochemical implications, which can influence biological activity, reactivity, and physical properties.

Implications of Proper Nomenclature in Scientific Contexts

1. Biological and Pharmacological Significance

Enantiomers often differ in how they interact with biological systems. For example, one enantiomer may be therapeutically active, while the other is inactive or even harmful. Precise IUPAC naming ensures clear communication in pharmacology.

2. Synthesis and Separation

In chemical synthesis, stereoselectivity is critical. Knowing the exact stereochemical configuration guides the design of synthetic pathways to obtain the desired enantiomer. Accurate nomenclature aids in reporting and reproducibility.

3. Regulatory and Patent Considerations

Legal and patent documents often specify stereochemistry explicitly. Precise IUPAC names prevent ambiguity and legal disputes.

Conclusion: The Primacy of Accurate Chemical Nomenclature

The comprehensive understanding of the IUPAC names for (1R,3R)-1-ethyl-3-methylcyclohexane and (1S,3S)-1-ethyl-3-methylcyclohexane underscores the importance of stereochemistry in organic chemistry. These compounds exemplify how three-dimensional arrangements influence naming, and consequently, their physical, chemical, and biological behavior.

Accurate naming facilitates effective communication, promotes clarity in scientific research, and underpins advances in medicine, materials science, and chemical synthesis. As chemists continue to explore complex molecules, mastery over IUPAC nomenclature remains a fundamental skill—serving as the language that unites the global scientific community in understanding molecular architecture.

In summary:

- The compounds are named based on the cyclohexane ring with substituents at carbons 1 and 3.
- The stereochemistry at each chiral center is explicitly indicated as R or S.
- The compounds are enantiomers, distinguished by their stereochemical configurations.
- The correct IUPAC names are (1R,3R)-1-ethyl-3-methylcyclohexane and (1S,3S)-1-ethyl-3-methylcyclohexane.

Understanding these principles ensures precise communication and advances in chemical sciences, reinforcing the critical role of nomenclature in the ever-evolving landscape of organic chemistry.

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