Deduce The Identity Of The Following Compound From The Spectral Data Given. C5h 100:1h Nmr, 8 1.2 (6h,

Deduce The Identity Of The Following Compound From The Spectral Data Given. C5H10:1H NMR, δ 8 1.2 (6H, s)

Introduction

Understanding the structure of organic compounds based on spectral data is a fundamental skill in organic chemistry. In this article, we will analyze the given spectral data to deduce the molecular identity of a compound with the formula C5H10, accompanied by specific NMR signals: a proton NMR (^{1}H NMR) signal at δ 1.2 integrating for six protons, appearing as a singlet (s). This process involves interpreting the molecular formula, the NMR chemical shift, integration, and splitting pattern to arrive at the most probable structure.

Understanding the Spectral Data

Molecular Formula: C5H10

- Degree of Unsaturation: The formula C5H10 suggests the compound is either a cycloalkane (ring structure) or an acyclic alkene with saturated carbons.
- Possible Structures:
- Cyclopentane
- Methylcyclopentane
- 1- or 2-pentene (alkenes)
- Isomers with different branching patterns

^{1}H NMR Data: δ 8 1.2 (6H, s)

- Chemical Shift (δ 1.2): Typical for alkyl protons (methyl or methylene groups attached to saturated carbons).
- Integration (6H): Six protons correspond to two methyl groups or a total of six equivalent hydrogens.
- Splitting Pattern (s): Singlet indicates these protons are equivalent and not coupled to neighboring hydrogens.

The key point here is that a singlet at δ 1.2 integrating for six protons suggests two equivalent methyl groups attached to a quaternary carbon or in an environment where protons are equivalent and not coupled to neighboring hydrogens.

Analyzing Possible Structures

1. Cyclopentane

- Structure: A five-membered saturated ring.
- NMR Expectation:
- All hydrogens are equivalent or nearly equivalent.
- Typically, methyl groups attached to the ring would resonate around δ 0.9–1.5 ppm.
- No methyl groups are explicitly attached; instead, hydrogens are on the ring carbons.

- Integration & Splitting:
- Hydrogens on cyclopentane usually appear as a multiplet due to ring strain and coupling.
- No methyl singlet at δ 1.2 integrating for six hydrogens is expected.

Hence, cyclopentane alone does not fit the spectral data.

2. Methyl-Substituted Cyclopentane (e.g., Methylcyclopentane)

- Structure: A cyclopentane ring with a methyl group attached.
- Expected NMR:
- Methyl attached to a quaternary or secondary carbon would appear as a singlet or multiplet around δ 0.9–1.2 ppm.
- The methyl group attached to the ring would give a singlet integrating for 3H.
- Additional methyl groups attached to the ring would give similar signals.

However, the spectral data shows a single singlet integrating for 6H, which suggests two equivalent methyl groups.

3. Dimethyl-Substituted Cyclic or Acyclic Structures

- Possible Structures:
- An acyclic alkane with two methyl groups attached to a quaternary carbon (e.g., neopentane).
- A cycloalkane with two methyl groups attached symmetrically.

Focusing on the Most Probable Structure

Given the data, the most consistent structure is 2,2-dimethylpropane (neopentane), but this has the formula C5H12, which is more saturated than C5H10. Therefore, it's not suitable unless we consider an unsaturation (alkene) or ring.

Alternatively, consider methylcyclopentane:

- Molecular formula matches C5H10.
- Two methyl groups attached at the same or different positions.
- The methyl groups attached to the ring would give a singlet if they are equivalent (symmetrical substitution).

But, the key is the spectral data: a singlet at δ 1.2 ppm integrating for six protons suggests two equivalent methyl groups attached to a quaternary carbon or in an environment where the two methyl groups are chemically equivalent and not split by neighboring hydrogens.

Therefore, the most likely structure is 2,2-dimethylcyclopentane.

Confirming with Structural Logic:
- 2,2-Dimethylcyclopentane has:
- Molecular formula: C5H10 (cyclopentane ring + two methyl groups)
- Symmetrical substitution at the second carbon.
- The methyl groups attached to the same carbon are equivalent.
- The methyl groups appear as a singlet in ^{1}H NMR at δ ~1.2 ppm, integrating for 6H.

Conclusion: The Identified Compound

Based on spectral data and structural reasoning, the compound is 2,2-dimethylcyclopentane.

Summary of Key Features:
- Molecular formula: C5H10
- NMR signal: δ 1.2 ppm, singlet, 6H
- Structure: A cyclopentane ring with two methyl groups attached to the same carbon (the second carbon), making it symmetrical and consistent with spectral data.

Additional Insights and Spectral Data Interpretation

Supporting Spectral Techniques

While only ^{1}H NMR data is provided, complementary spectral methods can further confirm the structure:

- **^{13}C NMR:** Would show signals for carbons in the ring and methyl groups.
- **Infrared (IR) Spectroscopy:** Would lack significant peaks for C=O or O-H, consistent with an alkane.
- **Mass Spectrometry:** The molecular ion peak at m/z 70 (C5H10) supports the molecular formula.

Implications for Organic Chemistry

Understanding how spectral data correlates with molecular structure is crucial for organic synthesis, compound identification, and purity assessment. The ability to interpret NMR signals, especially chemical shifts, integrations, and splitting patterns, allows chemists to distinguish between isomers and confirm molecular frameworks confidently.

Final Remarks

In conclusion, the spectral data of δ 1.2 ppm (6H, s) in the ^{1}H NMR spectrum of a compound with the molecular formula C5H10 strongly indicates the presence of two equivalent methyl groups attached to a quaternary carbon within a cyclic structure. The most consistent and logical structure matching all data points is 2,2-dimethylcyclopentane. This deduction exemplifies the critical role of NMR spectroscopy in structure elucidation and demonstrates the importance of integrating spectral data with chemical knowledge for accurate compound identification.

Keywords: spectral data, NMR, chemical shift, integration, C5H10, structure elucidation, 2,2-dimethylcyclopentane, organic chemistry, compound identification

Frequently Asked Questions

What information can be obtained from the C5H10 spectral data in NMR analysis?

The C5H10 spectral data provides insights into the number of hydrogen environments, their chemical shifts, and splitting patterns, which help identify the structure of the compound, such as whether it is cyclic or acyclic, and the types of hydrogens present.

How does the chemical shift at around 1.2 ppm assist in deducing the compound's structure?

A chemical shift at approximately 1.2 ppm typically indicates methyl groups attached to saturated carbons, suggesting the presence of alkyl chains or methyl substituents in the compound.

What does the integration value '6H' in the NMR spectrum suggest about the compound?

An integration of 6 hydrogens suggests the presence of two equivalent methyl groups or a methyl group with neighboring equivalent hydrogens, indicating symmetry or specific substituents in the molecule.

Can the multiplicity of the signal help determine the structure? If so, how?

Yes, the splitting pattern (such as triplet, doublet, singlet) indicates the number of neighboring hydrogens, which helps infer the connectivity and arrangement of groups within the molecule.

Based on the provided spectral data, what are the possible structural features of the compound?

The data suggests a saturated hydrocarbon with methyl groups, possibly an alkyl chain or cyclic structure with methyl substitutions, given the chemical shift and integration values.

How can the molecular formula C5H10 be used to narrow down the compound's identity?

The molecular formula indicates the compound is an alkene or cycloalkane with five carbons, and combined with NMR data, helps distinguish between different isomers such as cyclopentane or pentene derivatives.

What additional spectral data would help confirm the compound's identity?

Additional data like IR spectra (to identify functional groups), mass spectrometry (to confirm molecular weight), and 13C NMR would provide more comprehensive structural information.

Based on the spectral data provided, what is the most likely identity of the compound?

The compound is most likely cyclopentane, as it fits the molecular formula C5H10, and the NMR data indicating methyl groups with chemical shifts around 1.2 ppm, consistent with a saturated cyclic structure.

Additional Resources

Deduce The Identity Of The Following Compound From The Spectral Data Given: A Comprehensive Analytical Approach

In the realm of organic chemistry, the process of elucidating a compound's structure based solely on spectral data is both an art and a science. The ability to interpret NMR spectra, IR readings, mass spectra, and other spectroscopic data is fundamental for chemists engaged in structural determination. This investigative article aims to exemplify this process through a detailed analysis of a hypothetical compound, C_5H_{10}, provided with specific NMR data: a proton NMR signal at δ 1.2 ppm integrating to six hydrogens, with splitting indicating a triplet, suggestive of methyl groups attached to a methylene chain. Our goal is to deduce the identity of this compound systematically, highlighting the reasoning steps, spectral interpretation, and logical deductions involved.

Introduction: The Significance of Spectral Data in Structure Elucidation

Spectroscopy serves as the chemist's window into the molecular world. Among the various techniques, Nuclear Magnetic Resonance (NMR) spectroscopy is particularly powerful for determining the environment of hydrogen atoms in organic molecules. When combined with molecular formula data, spectral peaks, and splitting patterns, NMR can often lead to a definitive structure.

Given the molecular formula C_5H_{10}, the compound is an alkene or cycloalkane, or possibly an acyclic alkane with branches or rings. The spectral data provided is:

- Proton NMR: δ 1.2 ppm
- Integration: 6H
- Splitting: Triplet

This information suggests a methyl group (or groups) coupled to a neighboring methylene, characteristic of a $-CH_3-CH_2-$ fragment.

Understanding the Molecular Formula: C_5H_{10}

Before delving into the spectral data, it's essential to analyze the molecular formula:

- Degree of Unsaturation (Double Bond Equivalent, DBE):

$$
\text{DBE} = C - \frac{H}{2} + 1 = 5 - \frac{10}{2} + 1 = 5 - 5 + 1 = 1
$$

A DBE of 1 indicates either one double bond or a ring. Therefore, the compound is either:

- An alkene (with a C=C bond)
- A cycloalkane (a ring structure)

Interpreting the NMR Data

The key NMR features are:

- A signal at δ 1.2 ppm
- Integration: 6 hydrogens
- Multiplicity: triplet

Implications:

- The chemical shift at δ 1.2 ppm falls within the typical region for methyl groups attached to sp^3 carbons.
- The integration of 6H suggests two equivalent methyl groups, or a methyl group in a symmetrical environment.
- The triplet splitting indicates that these hydrogens are coupled to neighboring methylene hydrogens ($-CH_2-$), which typically produce a quartet if the coupling is with a methyl, but in this case, the observed triplet suggests the methyls are coupled to a $-CH_2-$ group.

Given this, the simplest fragment consistent with this NMR pattern is an ethyl group ($-CH_2-CH_3$).

Constructing Possible Structures

Combining the molecular formula and spectral clues, the following possibilities emerge:

1. An Alkene with an Ethyl Substituent

- The molecule could be an alkene with an ethyl group attached, e.g., butene derivatives.

2. A Cyclic Compound with an Ethyl Substituent

- A cyclopentane ring with an ethyl substituent, considering the degree of unsaturation.

3. An Alkyl Chain with a Double Bond

- For example, pentenes.

Let's analyze each possibility in detail.

Case 1: Alkene with an Ethyl Group

Possible structure: 1-ethyl-1-butene or similar.

- The ethyl group would give a triplet at δ 1.2 ppm integrating to 3H (methyl), and a quartet at δ ~2.0 ppm for the methylene attached to the double bond.

- But since the data shows only one peak at δ 1.2 ppm, and no mention of other signals, this scenario seems less likely unless the other signals are absent or overlapped.

Case 2: Cyclopentane with an Ethyl Substituent

- Cyclopentane (C_5H_{10}) itself has a saturated ring, but the spectral data suggests a substituent.

- If the compound is cyclopentane with an ethyl substituent, the total formula would be C_6H_{12}, which contradicts our initial formula.

- Alternatively, if the compound is a cyclopentene derivative, the formula would change; thus, this seems inconsistent.

Case 3: A Straight-Chain Alkene with a Methyl Substituent

- For example, 2-methyl-1-butene or 2-methyl-2-butene.

- These structures may fit the molecular formula, but the NMR data must be compatible.

Refining the Deduction: Focus on the NMR and Molecular Formula

The key clues are:

- The presence of a triplet at δ 1.2 ppm integrating to 6H.

- The splitting pattern indicates two equivalent methyl groups attached to a methylene.

- The molecular formula suggests one double bond or ring.

Given that, the most plausible structure is an ethyl group attached to an alkene or a ring.

Proposed Candidate: 1-Butene with an Ethyl Substituent

Let's consider but-1-ene ($CH_2=CH-CH_2-CH_3$):

- Total hydrogens: 8, so it does not match.

Next, 2-methyl-1-propene:

- Not matching the formula either.

Alternatively, pentene structures:

- 1-pentene: $CH_2=CH-CH_2-CH_2-CH_3$ (H count: 10; matches formula C_5H_{10})

- NMR for 1-pentene:

- The terminal methyl attached to the double bond appears as a triplet around δ 0.9 ppm.

- The methyl attached to the chain appears around δ 0.9–1.0 ppm.

- The chain methyls and methylenes appear between δ 1.2–2.0 ppm.

- But the observed data shows a single signal at δ 1.2 ppm for 6 hydrogens, which suggests the presence of

two methyl groups in similar environment.

Final Deduction: The Most Consistent Structure

Based on the spectral data—specifically, a triplet at δ 1.2 ppm integrating to 6H—the compound is most consistent with an ethyl group attached to a cyclopentane ring.

However, since the molecular formula is C_5H_{10}, and a cyclopentane with an ethyl substituent would be C_6H_{12}, this is not possible.

Alternatively, the data suggests the compound is pentane, with the methyl groups attached to a common methylene, or a branched chain.

The key is the triplet at δ 1.2 ppm (6H). In typical NMR spectra:

- Methyl groups attached to a methylene ($-CH_2-CH_3$) produce a triplet for methyls and a quartet for methylenes.

- The fact that only a triplet is observed suggests the methyl groups are terminal and equivalent.

Given all these considerations, the most straightforward structure fitting the spectral data and molecular formula is:

n-Butane ($CH_3-CH_2-CH_2-CH_3$)

- Total hydrogens: 10

- NMR:

- Terminal methyl groups appear as triplets at δ 0.9 ppm, integrating to 3H each.

- The methylene in the middle appears as a multiplet or a sextet, but if the spectrum is simplified, the methyls could appear as a triplet.

- The observed data: a single triplet at δ 1.2 ppm integrating to 6H suggests overlapping methyl signals.

But: The problem states the spectral data as δ 1.2 ppm (6H, triplet). If only this signal is observed, it indicates two methyl groups in similar environment, adjacent to a methylene.

Therefore, the most consistent structure is:

2,3-Dimethylbutane (Isopentane)

- Structural formula: $(CH_3)_2CH-CH_2-CH_3$

- But this has a different formula: C_5H_{12}.

- So, it is inconsistent with the given formula.

Conclusion: The Likely Identity

Based on the spectral data:

- Molecular formula: C_5H_{10} (degree of unsaturation: 1)

- NMR data: δ 1.2 ppm, 6H, triplet

The best fit is pent-1-ene

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