Deduce The Structure Of An Unknown Compound Using The Data.C5H10O: NMR: ???? 9.8 (1H, S), ???? 1.1 (9H,

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Introduction

Understanding the structure of an unknown organic compound is a fundamental task in organic chemistry. Spectroscopic techniques, especially Nuclear Magnetic Resonance (NMR) spectroscopy, provide invaluable insights into molecular frameworks. In this case, we are given the molecular formula $C_5H_{10}O$ and partial NMR data: a singlet at 9.8 ppm integrating for 1 proton and a signal at 1.1 ppm integrating for 9 protons. This guide aims to systematically analyze the data to deduce the compound's structure.

Analyzing the Molecular Formula: $C_5H_{10}O$

Before delving into NMR data, understanding the molecular formula helps narrow down possible structures.

Degree of Unsaturation

The degree of unsaturation (also called double bond equivalents, DBE) indicates the number of rings and/or multiple bonds:

1. Calculate: DBE = (2C + 2 + N - H - X)/2
2. Here, N and X (halogens) are zero, so:

   DBE = (2×5 + 2 - 10)/2 = (10 + 2 - 10)/2 = 2/2 = 1

This suggests the molecule contains either one double bond or one ring.

Implications of the Formula

- The presence of oxygen typically indicates an alcohol, aldehyde, ketone, ether, or ester.
- The molecular formula is consistent with several functional groups, but considering the NMR data (which you'll see below), we can narrow this further.

Interpreting the NMR Data

The key data points are:

- 9.8 ppm (1H, singlet)
- 1.1 ppm (9H, likely a triplet or multiplet, but here described as a signal for 9 protons)

Analysis of the 9.8 ppm Signal

- Chemical shift at 9.8 ppm is highly deshielded.
- Typical for aldehyde protons (–CHO), which resonate around 9.5 – 10 ppm.
- The singlet multiplicity suggests a proton attached to a carbon with no neighboring hydrogens—consistent with aldehyde.

Analysis of the 1.1 ppm Signal

- A signal at approximately 1.1 ppm integrating for 9 protons strongly suggests a tert-butyl group (–$C(CH_3)_3$).
- The chemical shift aligns with methyl groups attached to sp^3 carbons.

Summary of NMR Data Interpretation

- The presence of an aldehyde group (due to the 9.8 ppm singlet).
- The presence of a tert-butyl group (due to the 1.1 ppm integration).

Piecing Together the Structure

Given the above, we can hypothesize:

- The molecule contains an aldehyde functional group.
- It also contains a tert-butyl group.
- The molecular formula $C_5H_{10}O$ matches these features.

Possible Structural Frameworks

Considering the molecular formula and the NMR data, plausible structures include:

1. Aliphatic aldehyde with a tert-butyl substituent attached to the aldehyde carbon.
2. Acyclic structures with a tert-butyl group attached to a chain that ends with an aldehyde.

Proposed Structure: 2-Methyl-2-oxopropanal (or similar)

Based on the data, a reasonable structure is tert-butyl aldehyde (tert-butanal), which is C_4H_9CHO, but this molecule's formula is C_4H_9CHO (which matches $C_4H_{10}O$), so perhaps the structure is:

2,2-Dimethylpropanal (also known as tert-butyl aldehyde).

- The molecule: $(CH_3)_3C–CHO$
- Formula: $C_5H_{10}O$
- NMR data:
- Aldehyde proton at around 9.8 ppm (singlet, 1H)
- Tert-butyl group (nine methyl protons) at around 1.1 ppm

Structural features:

- The aldehyde group attached to a quaternary carbon.
- The quaternary carbon bears three methyl groups (tert-butyl group).

Confirmation of the Proposed Structure

The proposed structure aligns well with all observed data:

- Molecular formula: $C_5H_{10}O$
- Degree of unsaturation: 1 (aldehyde carbonyl)
- NMR signals:
- 9.8 ppm (singlet, 1H): aldehyde proton
- 1.1 ppm (9H): tert-butyl methyl groups

Additional Spectroscopic Considerations

To further confirm the structure, other spectroscopic techniques can be employed:

Infrared (IR) Spectroscopy

- Look for a strong absorption around 1720–1740 cm^{-1} characteristic of aldehyde C=O stretch.
- A C–H stretch near 2700–2900 cm^{-1} for aldehyde.

Mass Spectrometry (MS)

- Molecular ion peak at m/z corresponding to $C_5H_{10}O$ (which is 86 g/mol).
- Fragmentation patterns supporting the aldehyde and tert-butyl groups.

NMR Chemical Shifts in Detail

- The aldehyde proton appears downfield due to the electron-withdrawing carbonyl group.
- The tert-butyl methyl groups are shielded, resonating around 1.1 ppm.

Conclusion

By systematically analyzing the molecular formula and NMR data, the structure of the unknown compound $C_5H_{10}O$ with signals at 9.8 ppm (1H, singlet) and 1.1 ppm (9H) is most consistent with tert-butyl aldehyde (t-butanal). The aldehyde's proton resonates at approximately 9.8 ppm, and the tert-butyl group's nine methyl protons resonate at about 1.1 ppm. The structure features a quaternary carbon attached to an aldehyde group and three methyl groups, satisfying both the molecular formula and spectroscopic data.

This example illustrates how spectral data, combined with chemical reasoning, enables chemists to deduce molecular structures efficiently and accurately.

Keywords: Organic chemistry, NMR spectroscopy, molecular structure, aldehyde, tert-butyl, spectral analysis, $C_5H_{10}O$, structural elucidation

Frequently Asked Questions

What does the NMR signal at 9.8 ppm indicate in the compound C5H10O?

The signal at 9.8 ppm suggests the presence of an aldehyde proton, indicating an aldehyde functional group in the compound.

What does the singlet integrating to 9H at around 1.1 ppm imply about the structure?

A singlet integrating to 9H typically indicates three equivalent methyl groups, likely attached to a quaternary carbon or as tert-butyl groups.

Based on the NMR data, what functional groups are likely present in C5H10O?

The data suggests the presence of an aldehyde group (from the 9.8 ppm signal) and alkyl groups (from the 1.1 ppm signal), indicating a structure that includes an aldehyde and possibly a tert-butyl or similar alkyl substituents.

How can the molecular formula C5H10O help in deducing the compound's structure?

The formula indicates five carbons, ten hydrogens, and one oxygen atom, consistent with aldehydes, ketones, or alcohols; combined with NMR data, it helps narrow down possible structures such as aldehyde derivatives with bulky alkyl groups.

What type of compound could have a singlet at 1.1 ppm integrating to 9H and an aldehyde proton at 9.8 ppm?

This pattern is characteristic of a tert-butyl aldehyde or related structure where a tert-butyl group (9H) is attached to an aldehyde functional group.

What additional spectroscopic data would help confirm the structure of the compound?

Infrared (IR) spectroscopy to identify characteristic carbonyl stretching, and 13C NMR to determine carbon environments, would help confirm the presence of aldehyde and alkyl groups, solidifying the compound's structure.

Additional Resources

Deduce the Structure of an Unknown Compound Using the Data $C_5H_{10}O$: A Comprehensive Analysis

Understanding the structure of an unknown organic compound based solely on its molecular formula and spectroscopic data is a fundamental skill in organic chemistry. The

molecular formula $C_5H_{10}O$ indicates a degree of unsaturation and possible functional groups, but it leaves many structural possibilities open. Here, we will systematically analyze the provided data and apply various spectroscopic principles to deduce the most probable structure, focusing especially on the NMR data.

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1. Molecular Formula and Initial Considerations

1.1. Calculating Degree of Unsaturation

Given the molecular formula:

- $C_5H_{10}O$

The degree of unsaturation (also called double bond equivalents, DBE) can be calculated using the formula:

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

Since there are no nitrogen atoms:

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

Thus, the molecule contains one degree of unsaturation, which could be:

- A double bond (alkene),
- A ring (cyclic structure),
- Or a triple bond (less likely here because of the hydrogen count, but possible).

Given the hydrogen count and the presence of oxygen, the most common possibilities include:

- A cyclic structure with a single double bond or a carbonyl group,
- An acyclic structure with a double bond or an oxygen in a functional group.

1.2. Functional Group Considerations

- The molecular formula suggests the presence of an oxygen atom, which could be part of:

- An alcohol (–OH),
- An ether (–O–),
- A carbonyl group (ketone, aldehyde, ester, or C=O),
- A cyclic ether.

- The molecular formula and degree of unsaturation imply the presence of either a carbonyl group or a double bond.

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2. Interpreting the NMR Data

The key to structural elucidation is the NMR data:

> NMR: ???? 9.8 (1H, S), ???? 1.1 (9H,)

2.1. Analyzing the Proton at 9.8 ppm (1H, Singlet)

- Chemical Shift (~9.8 ppm): Indicates a highly deshielded proton, typical of:

- An aldehyde proton (–CHO) usually appears between 9.0–10.0 ppm,
- An acidic proton (e.g., carboxylic acid) often appears around 10–12 ppm,
- Or an aromatic proton in certain cases, but the singlet and integration suggest otherwise.

- Singlet (S): Implies no coupling, typical for aldehyde protons because they usually don't have adjacent hydrogens to couple with.

Conclusion: The 9.8 ppm singlet likely corresponds to an aldehyde proton.

2.2. Analyzing the Proton at 1.1 ppm (9H, bolded keyword)

- Chemical Shift (~1.1 ppm): Typical of methyl groups (–CH_3) attached to saturated carbons.

- Integration (9H): Indicates three methyl groups.

- Possible interpretations:

- A tert-butyl group ($\text{(CH}_3)_3\text{C}$) has 9 protons, all equivalent, appearing as a singlet at around 1.0–1.2 ppm.

- Alternatively, three methyl groups attached to different parts of the molecule, but the high symmetry and the singlet suggest a tert-butyl group.

Conclusion: The 1.1 ppm signal with 9H integration suggests the presence of a tert-butyl group.

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3. Deductive Reasoning for Structural Features

3.1. Summarizing Spectroscopic Clues

- Presence of an aldehyde group: Implied by the 9.8 ppm singlet (1H).
- Presence of a tert-butyl group: Indicated by the 1.1 ppm (9H, s).
- Molecular formula: $C_5H_{10}O$.

3.2. Compatibility of Functional Groups

- The aldehyde (–CHO) is typically attached to an sp^2 carbon, often in a terminal position.
- The tert-butyl group is bulky and usually attached to a carbon chain or to a carbonyl carbon in esters or ketones.

3.3. Possible Structural Motifs

- Aldehyde with a tert-butyl group attached directly: Unlikely because the molecular formula would then be inconsistent unless the chain length and substituents match.

- Aldehyde attached to a tert-butyl substituent: For example, a tert-butyl aldehyde (p-tolualdehyde) would have more carbons.

- Aldehyde adjacent to an ether or alcohol group: Less likely given the formula.

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4. Building Candidate Structures

Given the clues, the most plausible candidate is an aldehyde with a tert-butyl substituent.

4.1. Candidate 1: 2-Methylpropionaldehyde (isobutyraldehyde)

- Structure:

```
CH3
|
CH3–CH–CHO
```

- Molecular formula check:

- 4 carbons in total, but our formula requires 5 carbons, so this is inconsistent.

4.2. Candidate 2: 2,2-Dimethylpropanal (pivaldehyde)

- Structure:

```
CH3
|
(CH3)3C–CHO
```

- Number of carbons: 4 in tert-butyl + 1 in aldehyde = 5 carbons.

- Hydrogens:

- Tert-butyl: 9H

- Aldehyde proton: 1H

- Total hydrogens: 10

- Oxygen: in aldehyde group.

- Matching the formula: $C_5H_{10}O$.

- Spectroscopic data:

- The aldehyde proton at ~9.8 ppm (singlet): matches.

- The tert-butyl methyl groups: give a singlet at ~1.1 ppm integrating to 9H: matches.

Conclusion: The structure pivaldehyde (2,2-dimethylpropanal) fits the data well.

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5. Confirming the Structural Proposal

5.1. Chemical Shift Consistency

- Aldehyde proton (~9.8 ppm, singlet): typical for aldehydes.

- Methyl groups attached to quaternary carbon (tert-butyl): give a sharp singlet at around 1.1 ppm, integrating to 9H.

5.2. Additional Spectroscopic Considerations

- Additional NMR data (not provided): Would likely show:

- Carbon NMR signals consistent with the aldehyde carbon (~190–200 ppm).

- Quaternary carbon of tert-butyl at ~60–70 ppm.

- Methyl carbons at ~20 ppm.

- IR spectrum (not provided): Would show a strong aldehyde C=O stretch (~1725 cm^{-1}).

5.3. Structural Implications

- The quaternary carbon bearing the three methyl groups is attached directly to the aldehyde carbon, making the structure compact and consistent with all data.

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6. Final Structural Deduction

The most consistent and plausible structure for $C_5H_{10}O$, based on the given NMR data, molecular formula, and chemical reasoning, is:

Pivaldehyde (2,2-dimethylpropanal)

Structural formula:

```
CHO
|
(CH3)3C
```

- The aldehyde group at the end of a tert-butyl group.

- The methyl groups on the quaternary carbon give rise to the 1.1 ppm (9H, s) signal.

- The aldehyde proton at 9.8 ppm (s) is characteristic of aldehyde hydrogens.

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7. Broader Implications and Additional Confirmations

7.1. Importance of Complementary Data

While the NMR data strongly suggest pivaldehyde, confirming with additional spectroscopic techniques enhances confidence:

- Infrared (IR) spectroscopy: Presence of a sharp aldehyde C=O stretch (~1725 cm^{-1}).

- Mass spectrometry (MS): Molecular ion peak at m/z 86 (consistent with $C_5H_{10}O$), with fragmentation patterns characteristic of aldehydes.

- Carbon NMR (^{13}C NMR): Aldeh

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