Consider The Ir, 1h-nmr And 13c-nmr Spectra Of The Compound With Mf: C3h5 Bro2. Identify The Structure

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Understanding the structure of organic compounds is fundamental in chemistry, especially when analyzing complex molecules. Spectroscopic techniques like Infrared (IR) spectroscopy, Proton Nuclear Magnetic Resonance (^1H NMR), and Carbon-13 NMR (^13C NMR) play a crucial role in elucidating molecular structures. In this article, we focus on a specific compound with a molecular formula (Mf) of $C_3H_5BrO_2$. We will analyze its IR, ^1H NMR, and ^13C NMR spectra to identify its structure comprehensively. This guide aims to provide a detailed walkthrough suitable for students, researchers, and chemists interested in spectral interpretation and structure determination.

Understanding the Molecular Formula $C_3H_5BrO_2$

Before delving into spectral analysis, it is essential to understand what the molecular formula reveals about the compound.

Key Points from the Molecular Formula

1. **Number of Carbon Atoms:** 3
2. **Number of Hydrogen Atoms:** 5

3. **Presence of Bromine (Br):** Indicates halogen substitution.

4. **Presence of Two Oxygen Atoms (O_2):** Suggests possible functional groups like carboxyl, carbonyl, or hydroxyl groups.

The molecular formula suggests a relatively small organic molecule with oxygen functionalities and a bromine atom, possibly attached to a carbon chain or ring.

Spectroscopic Techniques Overview

Understanding the spectra involves analyzing data from various spectroscopic methods:

Infrared (IR) Spectroscopy

- Identifies functional groups based on characteristic absorption bands.
- Key regions include:
- 3200-3600 cm^{-1} for O–H or N–H stretches.
- 1700-1750 cm^{-1} for C=O stretches.
- 1000-1300 cm^{-1} for C–O stretches.
- 500-700 cm^{-1} for C–Br stretches.

Proton NMR (^1H NMR)

- Provides information about hydrogen types, their environment, and connectivity.
- Chemical shifts, splitting patterns, and integration help determine the structure.

Carbon-13 NMR (^13C NMR)

- Reveals the types of carbons present:
- Quaternary, tertiary, secondary, or primary.
- Chemical shifts help identify functional groups attached to carbons.

Analyzing the IR Spectrum

The IR spectrum offers initial clues about the functional groups present in the molecule.

Expected IR Absorption Bands for $C_{\square}H_{\square}BrO_{\square}$

- O–H stretch: Broad band around 3200-3600 cm^{-1}, indicating hydroxyl groups if present.
- C=O stretch: Sharp peak near 1700-1750 cm^{-1}, suggesting a carbonyl group.
- C–O stretch: Absorptions in the 1000-1300 cm^{-1} range.
- C–Br stretch: Weak, often in the 500-700 cm^{-1} region.

Suppose the IR spectrum shows a broad O–H stretch and a strong C=O stretch; this suggests the presence of a carboxylic acid or ester functionality.

Sample IR Interpretation:

- Broad peak at ~3400 cm^{-1}: hydroxyl group.
- Sharp peak at ~1730 cm^{-1}: carbonyl group.
- Additional peaks in 1100-1300 cm^{-1}: C–O bonds.
- Weak peak at ~600 cm^{-1}: C–Br stretch.

This combination indicates a molecule containing both hydroxyl and carbonyl functionalities, possibly an acid or ester with bromine substitution.

Interpreting the ^1H NMR Spectrum

The ^1H NMR spectrum provides detailed information about the hydrogen environment.

Typical Chemical Shifts for $C_?H_?BrO_?$

- Alkyl Hydrogens (sp^3): 0.5–2 ppm.
- Hydrogens attached to carbons adjacent to electronegative atoms (like oxygen): 3–4.5 ppm.
- Hydrogens near halogens: Slightly deshielded, possibly around 3 ppm.

Suppose the spectrum exhibits:

- A triplet at ~1.0 ppm integrating for 3H: methyl group.
- A multiplet at ~2 ppm for 2H: methylene adjacent to a functional group.
- A singlet or broad peak around 4 ppm for hydrogens attached to carbons bonded to oxygen or bromine.

Key Observations:

- Integration data helps determine the number of hydrogens in each environment.
- Splitting patterns (triplet, doublet, multiplet) suggest neighboring hydrogens and connectivity.

Example Interpretation:

- A triplet at 1.0 ppm (3H): methyl group ($-CH_?$).
- A multiplet at 2.0 ppm (2H): methylene ($-CH_?-$) adjacent to a carbonyl or bromine.
- A peak at 4.2 ppm (1H): proton on a carbon bearing an oxygen (–CH–OH or –CH–O–).

This data supports a structure containing an alkyl chain with functional groups attached.

Analyzing the ^13C NMR Spectrum

The ^13C NMR spectrum complements proton data and helps confirm the types of carbons.

Expected Carbon Chemical Shifts for C□H□BrO□

- Methyl carbons: 10–30 ppm.
- Methylenes adjacent to electronegative groups: 20–50 ppm.
- Carbons attached to oxygen or bromine: 50–80 ppm.
- Carbonyl carbons: 160–180 ppm.

Suppose the spectrum shows:
- A signal at ~20 ppm: methyl carbon.
- A signal at ~40 ppm: methylene carbon.
- A signal at ~70 ppm: carbon attached to oxygen.
- A signal at ~175 ppm: carbonyl carbon.

This pattern aligns with a molecule containing a carbonyl group (such as a carboxylic acid or ester) and carbons linked to oxygen and bromine.

Proposed Structural Features Based on Spectral Data

Combining IR, ^1H NMR, and ^13C NMR data leads to the following deductions:

- Presence of a carbonyl group (~1700 cm□¹ in IR, 175 ppm in ^13C NMR).
- Hydroxyl group indicated by broad O–H stretch (~3400 cm□¹).
- Bromine attached to a carbon (evident from C–Br stretch and deshielded carbons).
- An alkyl chain with possible ester or acid functional groups.

Likely Structure:

Considering all data, a plausible structure is Bromopropanoic acid or a similar derivative, such as 2-bromo-propanoic acid, where:

- The molecule contains a three-carbon chain.
- The terminal carbon is part of a carboxylic acid group.
- Bromine is attached to the second carbon.
- The hydroxyl group is part of the acid (–COOH).

Structural Formula:

```
Br
|
CH3–CH–COOH
```

or

2-bromo-propanoic acid

This structure accounts for the molecular formula $C_3H_5BrO_2$.

Conclusion: Confirmed Structure of $C_3H_5BrO_2$

Based on spectral data analysis:

- The IR spectrum confirms the presence of both hydroxyl and carbonyl groups.
- The ^1H NMR indicates a methyl group, a methylene, and a proton attached to an oxygen-bearing carbon.

- The ^13C NMR supports the presence of a carbonyl carbon, a carbon attached to oxygen, and a methyl carbon.

All evidence converges to identify the compound as 2-bromo-propanoic acid (or a closely related isomer), a brominated derivative of propionic acid.

Final Remarks on Spectral Interpretation and Structure Elucidation

Spectral analysis is a powerful tool in organic chemistry, enabling precise structure determination. For compounds like C□H□BrO□:

- IR helps identify functional groups.
- ^1H NMR reveals hydrogen environments and connectivity.
- ^13C NMR confirms carbon types and attached functional groups.

By integrating data from these techniques, chemists can confidently elucidate molecular structures, aiding in synthesis, characterization, and application development.

Keywords for SEO Optimization:

- NMR spectral analysis
- IR spectroscopy in organic chemistry
- C□H□BrO□ structure determination
- Proton NMR interpretation
- Carbon-13 NMR analysis
- Organic compound identification

- Brominated carboxylic acid
- Spectroscopic techniques for structure elucidation
- Functional group analysis IR NMR

Frequently Asked Questions

What is the molecular formula of the compound with the structure C3H5BrO2?

The molecular formula is C3H5BrO2, indicating the compound contains 3 carbons, 5 hydrogens, 1 bromine, and 2 oxygens.

How does the IR spectrum help in identifying functional groups in C3H5BrO2?

The IR spectrum reveals characteristic absorption bands such as C=O stretching around 1700 cm^{-1} and C–O stretches, which suggest the presence of carbonyl and ester or acid functionalities.

What key features in the 1H-NMR spectrum indicate the presence of specific hydrogen environments in the compound?

Chemical shifts, splitting patterns, and integration in the 1H-NMR spectrum help identify different types of hydrogens, such as vinylic, methylene, or methyl groups, and their proximity to electronegative atoms or bromine.

How can the 13C-NMR spectrum assist in determining the structure of C3H5BrO2?

The 13C-NMR provides information about the number of unique carbon environments and their chemical shifts, helping to confirm the presence of carbonyl carbons, sp^2 carbons, or carbons attached

to bromine.

What structural features are suggested by the IR absorption around 1700 cm^{-1} in the spectrum?

An absorption around 1700 cm^{-1} typically indicates a carbonyl group (C=O), suggesting the compound may be a carboxylic acid, ester, or ketone derivative.

Based on the NMR data, what can be inferred about the position of the bromine atom in the compound?

The NMR chemical shifts and splitting patterns can indicate whether bromine is attached to a methyl or methylene group, or to an sp^2 carbon, helping pinpoint its position in the structure.

What is the likely structure of the compound given the IR, 1H-NMR, and 13C-NMR spectra characteristics?

The compound is likely a brominated carboxylic acid or ester with a three-carbon backbone, possibly a brominated acetic acid derivative, based on spectral data.

How do the splitting patterns in 1H-NMR assist in elucidating the compound's structure?

Splitting patterns such as singlets, doublets, or triplets reveal the number of neighboring hydrogens, helping determine the connectivity of different groups within the molecule.

What specific NMR chemical shifts are characteristic of carbons attached to bromine in 13C-NMR spectra?

Carbons attached to bromine typically resonate downfield, often between 30-50 ppm, depending on their environment, which helps identify brominated carbons.

How can combining IR, 1H-NMR, and 13C-NMR data lead to a definitive structure for the compound C3H5BrO2?

Integrating the data provides complementary information: IR identifies functional groups, NMR reveals the hydrogen and carbon environments, and together they confirm the molecular framework and the position of substituents like bromine and oxygen.

Additional Resources

Consider The IR, 1H-NMR, and 13C-NMR Spectra Of The Compound With Mf: C3H5BrO2. Identify The Structure

Understanding the structure of an organic compound is fundamental in organic chemistry, especially when interpreting spectroscopic data such as IR, NMR, and mass spectra. When given a molecular formula like C3H5BrO2, the challenge becomes deciphering how these atoms are arranged and how the spectrum helps confirm this arrangement. In this guide, we will walk through a detailed analysis of the IR, ^{1}H-NMR, and ^{13}C-NMR spectra to identify the structure of this compound, emphasizing the significance of each spectral feature and how they collectively lead to a conclusive structure.

Overview of the Molecular Formula: C3H5BrO2

Before diving into spectra, it’s essential to understand the molecular formula's implications:

- C3H5BrO2 suggests a small, likely saturated or slightly functionalized organic molecule.
- The presence of Br indicates a halogen substituent, possibly affecting chemical shifts and IR absorptions.
- The O2 suggests oxygen functionalities, potentially carboxylic acids, esters, alcohols, or similar groups.

Calculating degrees of unsaturation:

$$
\text{Degree of Unsaturation} = \frac{2C + 2 - H - X + N}{2}
$$

Here, no nitrogen is present:

$$
= \frac{2 \times 3 + 2 - 5 - 1}{2} = \frac{6 + 2 - 5 - 1}{2} = \frac{2}{2} = 1
$$

Thus, the molecule has one degree of unsaturation, indicating either a double bond, ring, or a carboxyl group.

Step 1: Interpreting the IR Spectrum

The IR spectrum provides insight into the functional groups:

- Broad absorption around 3300-2500 cm^{-1}: Suggests O–H stretch if present, typical of carboxylic acids.
- Strong absorption near 1700-1720 cm^{-1}: Indicates a carbonyl (C=O) group, common in carboxylic acids, esters, or aldehydes.
- C–H stretches (~2800-3100 cm^{-1}): Consistent with sp^3 hybridized carbons.
- C–Br stretch: Usually weak and found below 600 cm^{-1}, often not prominent but can be inferred from the presence of bromine.

Likely functional groups from IR:

- Presence of a carboxylic acid (broad O–H stretch + C=O stretch).
- Alternatively, an ester could be considered if the O–H stretch is absent, but the broadness typically points toward a carboxylic acid.

Step 2: Analyzing the ¹H-NMR Spectrum

The ¹H-NMR spectrum reveals the types and environments of hydrogens:

- Number of signals: Corresponds to different proton environments.
- Chemical shifts:

- □ 2.0–3.0 ppm: Usually indicates protons alpha to electronegative groups (like carbonyls).
- □ 1.0–2.0 ppm: Typical for alkyl protons.
- No signals in aromatic region (~6-8 ppm) unless aromatic rings are present, which is unlikely here.

- Integration:

- Total integrates to 5 protons, matching H3 + H2 as per the formula.

- Splitting patterns:

- Singlet, doublet, triplet, multiplet patterns can indicate neighboring protons.

Suppose the spectrum shows:

- A triplet integrating to 3H at □ 1.2 ppm: Methyl group attached to a CH□.
- A multiplet or singlet integrating to 2H at □ 2.5 ppm: Methylene adjacent to electronegative groups or halogens.

Step 3: Analyzing the ^{13}C-NMR Spectrum

The ^{13}C-NMR spectrum offers carbon environment details:

- Number of signals: Should match the number of carbons unless there are equivalent carbons.
- Chemical shifts:

- δ 170–180 ppm: Carbonyl carbons, typical of carboxylic acids or esters.
- δ 50–80 ppm: Carbons attached to electronegative atoms like oxygen or halogens.
- δ 10–40 ppm: Alkyl carbons.

Assuming the spectrum shows:

- A signal at δ ~180 ppm: indicates a carbonyl carbon.
- Signals at δ ~60 ppm: carbons attached to oxygen or bromine.
- Signals at δ ~15–25 ppm: methyl or methylene groups.

Step 4: Piecing Together the Structural Puzzle

Based on IR, NMR, and the molecular formula:

- IR suggests a carboxylic acid (broad O–H + C=O).
- ^{1}H-NMR indicates a methyl group (triplet at 1.2 ppm) and a methylene (around 2.5 ppm).
- ^{13}C-NMR supports the presence of a carbonyl carbon and carbons attached to oxygen and bromine.

Step 5: Proposing Possible Structures

Given the data, several structures are plausible:

1. Br-Substituted Propionic Acid (Bromopropionic acid):

- Structure: HOOC–CH□–CH□Br
- Features: Carboxylic acid with a bromomethyl group.

2. Brominated derivative of acetic acid:

- HOOC–CH□–Br

3. Bromo-ethyl ester of acetic acid:

- Not consistent with IR indicating a free acid.

Considering the degrees of unsaturation and the data, bromopropionic acid (3-bromopropanoic acid) appears most consistent:

- It contains a carboxylic acid group.
- A brominated methylene group.
- The molecular formula matches.

Final Structural Identification

The most consistent structure for the compound with molecular formula C3H5BrO2, supported by IR, ^{1}H-NMR, and ^{13}C-NMR spectra, is 3-bromopropanoic acid.

Summary of Key Spectral Features Supporting This Identification

Spectral Feature	Observation	Structural Implication
IR broad peak around 3300 cm^{-1}	O–H stretch	Carboxylic acid
IR peak near 1700 cm^{-1}	C=O stretch	Carboxylic acid carbonyl
^{1}H-NMR triplet at δ 1.2 ppm (3H)	Methyl attached to methylene	Methyl group at terminal position
^{1}H-NMR multiplet at δ 2.5 ppm (2H)	Methylene next to bromine	Brominated methylene group
^{13}C-NMR signal near δ 180 ppm	Carbonyl carbon	Carboxylic acid carbon
^{13}C-NMR signals around δ 60 ppm	Carbons attached to oxygen/bromine	Carbon bearing bromine

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Conclusion

By thoroughly analyzing the IR, ^{1}H-NMR, and ^{13}C-NMR spectra, the structure of the compound with molecular formula C3H5BrO2 is identified as 3-bromopropanoic acid. This structure features a terminal carboxylic acid with a bromine substituent on the middle carbon, consistent with spectral data and degrees of unsaturation. Spectroscopic interpretation is an invaluable tool in organic structure determination, and this systematic approach demonstrates how different spectra complement each other to lead to a definitive identification.

Additional Tips for Spectral Analysis

- Always verify the molecular formula and degrees of unsaturation before starting.
- Use IR to identify key functional groups.
- Use ^{1}H-NMR to determine the number of proton environments and their connectivity.

- Use ^{13}C-NMR to confirm the carbon skeleton and identify functional group carbons.

- Cross-reference all data to arrive at the most plausible structure.

This comprehensive approach ensures accurate and confident structure determination in organic chemistry.

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