A Compound With A Molecular Ion Peak At M/z = 106 Has A Strong Peak At 1739cm-1 In Its IR Spectrum. Determine

A Compound With A Molecular Ion Peak At M/z = 106 Has A Strong Peak At 1739cm-1 In Its IR Spectrum. Determine

Understanding the molecular structure and composition of organic compounds often involves analyzing various spectroscopic data. When provided with a molecular ion peak at m/z = 106 and a prominent IR absorption at 1739 cm-1, chemists can make educated deductions about the molecular formula and functional groups present in the compound. This article aims to guide you through the interpretative process, exploring how to determine the molecular structure based on these spectral clues.

Interpreting the Mass Spectrum: The Significance of M/z = 106

Understanding the Molecular Ion Peak

The molecular ion peak, often represented as M+, reflects the molecular weight of the entire neutral molecule. In this case, an M/z value of 106 suggests that the molecular weight of the compound is approximately 106 g/mol. This is a crucial starting point, as it limits the possible molecular formulas that the compound can have.

Calculating Possible Molecular Formulas

To determine the possible molecular formulas corresponding to a molecular weight of 106, chemists typically consider common elements found in organic compounds, primarily carbon (C), hydrogen (H), oxygen (O), nitrogen (N), and halogens (Cl, Br, etc.). Given the molecular weight, a logical step is to generate empirical formulas that fit this weight.

Common approaches include:

- Using molecular weight constraints: For example, a formula like $C_6H_{10}O$ would total:

- C (12.01 × 6) = 72.06

- H (1.008 × 10) = 10.08

- O (16.00) = 16.00

- Total: 98.14 g/mol, which is slightly less than 106.

- Adjusting the number of carbons and hydrogens: For example, $C_7H_{10}O$:

- C (84.07) + H (10.08) + O (16.00) = 110.15 g/mol, slightly over 106.

- Considering molecules with halogens or nitrogen: For example, $C_5H_{10}O_2$:

- C (60.05) + H (10.08) + O2 (32) = 102.13 g/mol, close but slightly under.

Likely molecular formula: Given these calculations, the most probable molecular formula for the compound with a molecular weight of 106 is $C_6H_{14}O$, C_7H_{14}, or similar, but further data are needed for confirmation.

Analyzing the IR Spectrum: The Significance of the Peak at 1739 cm^{-1}

IR Absorption and Functional Groups

Infrared (IR) spectroscopy provides insights into the functional groups present in a molecule based on characteristic absorption frequencies. The peak at 1739 cm-1 is particularly indicative of a carbonyl (C=O) group, as this region is typical for various carbonyl-containing compounds.

Key points:

- Peak at approximately 1735–1750 cm-1: Usually signifies a carbonyl group, such as in aldehydes, ketones, esters, or carboxylic acids.

- Peak intensity: A strong IR absorption suggests a significant presence or a non-conjugated carbonyl, which absorbs strongly in this region.

- Additional peaks: To further specify the compound, additional IR peaks should be considered, such as O–H (broad, around 3200–3600 cm-1), N–H (around 3300–3500 cm-1), or C–H stretches (around 2800–3100 cm-1), depending on the functional groups.

In this case, the key observation is the strong IR peak at 1739 cm-1, pointing towards a carbonyl group.

Deduction of the Compound's Structure

Combining the mass spectral data with IR absorption characteristics allows us to propose possible structures.

Possible Functional Groups

The IR data suggests the presence of a carbonyl group. The molecular weight (~106) and the IR peak are compatible with several functional groups:

- Ketones: Characterized by a C=O stretch around 1715–1750 cm-1. Often, ketones are secondary or tertiary, with no O–H or N–H.

- Aldehydes: Also show C=O peaks, slightly shifted depending on conjugation, typically near 1725–1740 cm-1.

- Esters: Display C=O stretches near 1735–1750 cm-1, often with additional C–O peaks around 1000–1300 cm-1.

- Carboxylic acids: Usually have broad O–H stretch overlapping with C=O, but the absence of a broad O–H signal may suggest otherwise.

Given the data, the compound is most likely a ketone or an aldehyde.

Matching Molecular Formula to Functional Group

Possible molecular formulas with C, H, and O elements fitting the molecular weight include:

- $C_6H_{10}O$ (molecular weight 98): Slightly under 106, but close.

- $C_7H_{14}O$ (molecular weight 114): Slightly over.

- $C_6H_{12}O_2$: Braiding more oxygen atoms.

- $C_5H_{10}O_2$: 102 g/mol.

The most compatible molecular formula based on the molecular weight and the IR data is $C_6H_{10}O$, which aligns with a ketone or aldehyde with six carbons.

An example compound: 2-Hexanone (a ketone with six carbons) has the molecular formula $C_6H_{12}O$. Its molecular weight is 100 g/mol, slightly below 106, so perhaps a methyl-substituted derivative.

Alternatively, butanal (butyraldehyde) has C_4H_8O, molecular weight 72, too low.

Hence, a logical candidate could be pentanal ($C_5H_{10}O$) with molecular weight 86, still below 106.

Thus, the potential structure is a six-carbon aldehyde or ketone, possibly with methyl substitutions to reach the molecular weight of 106.

Additional Spectroscopic and Analytical Techniques for Confirmation

While the spectral data provides valuable clues, definitive structural determination often requires multiple analytical techniques.

1. NMR Spectroscopy

- **Proton NMR (1H NMR): Helps identify the number and types of hydrogen environments, distinguishing between aldehyde, methyl, methylene, or aromatic hydrogens.**

- Carbon NMR (13C NMR): Clarifies the number of unique carbon atoms, especially useful for identifying carbonyl carbons.

2. Additional IR Peaks

- Check for other characteristic peaks:

- O–H stretch (around 3200–3600 cm-1) if carboxylic acids are present.

- C–H stretches (around 2800–3100 cm-1).

- C–O stretches (for esters or acids).

3. Mass Spectrometric Fragmentation Patterns

- Fragmentation can reveal the presence of specific groups, such as aldehyde or ketone fragments.

Conclusion: Summarizing the Deduction

By integrating the spectral data:

- The molecular ion peak at m/z = 106 indicates a molecular weight of approximately 106 g/mol.

- The IR peak at 1739 cm-1 suggests a carbonyl group, likely a ketone or aldehyde.

- The most probable molecular formula is C6H10O or similar variants, pointing toward a six-carbon aldehyde or ketone.

- The compound could be a methyl-substituted pentanal or hexanone.

- Further spectroscopic data, such as NMR, would refine the structure.

In summary, the compound is most likely a six-carbon

Frequently Asked Questions

What does a molecular ion peak at m/z = 106 indicate about the compound's molecular weight?

It suggests that the molecular weight of the compound is approximately 106 atomic mass units (amu).

What functional group typically shows a strong IR absorption around 1739 cm^{-1}?

A strong IR absorption at around 1739 cm^{-1} is characteristic of a carbonyl group (C=O), commonly found in aldehydes, ketones, carboxylic acids, and esters.

Given the molecular weight and IR data, what possible compound classes could this molecule belong to?

It could be a simple ketone, aldehyde, or ester, as these often have molecular weights near 106 and show a strong carbonyl absorption near 1739 cm^{-1}.

How can the molecular ion peak assist in determining the molecular formula of the compound?

The molecular ion peak provides the molecular weight, which, combined with isotopic patterns and other spectral data, helps deduce the molecular formula.

What additional spectral information would help confirm the structure of this compound?

NMR spectroscopy, especially ^{1}H and ^{13}C NMR, along with fragmentation patterns from MS and detailed IR analysis, would aid in confirming the structure.

Could the compound be an ester based on the IR and mass spectra data? Why or why not?

Yes, it could be an ester because esters have a carbonyl group absorbing near 1739 cm^{-1} and a molecular weight close to 106, but further spectral data is needed for confirmation.

What steps should be taken next to accurately identify this compound?

Perform further spectroscopic analyses such as NMR, MS fragmentation studies, and possibly UV-Vis spectra, to determine the compound's structure definitively.

Additional Resources

A Compound With A Molecular Ion Peak At M/z = 106 Has A Strong Peak At 1739cm-1 In Its IR Spectrum. Determine

Understanding the molecular identity of organic compounds often involves interpreting their spectroscopic data. In this context, a compound exhibiting a molecular ion peak at m/z = 106 in mass spectrometry and a prominent IR absorption at 1739 cm^{-1} presents an intriguing puzzle. This article delves into the analytical approach to deciphering such a compound, exploring the significance of each spectral feature, the likely structural motifs involved, and the logical reasoning that leads to a probable molecular identity. Through detailed analysis, we aim to demonstrate how these spectroscopic clues can be integrated to arrive at a confident structural deduction.

Mass Spectrometry: Interpreting the M/z = 106 Molecular Ion Peak

Mass spectrometry (MS) is a cornerstone technique for determining the molecular weight and, by extension, the molecular formula of organic compounds. The molecular ion peak, often denoted as [M]+•, corresponds to the intact molecule ionized but unfragmented, and its m/z value provides crucial information about the molecular mass.

Significance of the Molecular Ion Peak at m/z = 106

- Molecular Weight Estimate: The peak at m/z = 106 indicates that the molecular weight of the compound is approximately 106 amu (atomic mass units).
- Molecular Formula Constraints: Using the molecular weight, we can propose plausible molecular formulas that satisfy this weight while considering common elements in organic chemistry: carbon (C), hydrogen (H), oxygen (O), nitrogen (N), etc.

Establishing Possible Molecular Formulas

Given the mass of 106, potential formulas include:

- $C_6H_{10}O$: Molecular weight = (6×12.01) + (10×1.008) + (16.00) = 72.06 + 10.08 + 16.00 = 98.14 (too low)
- C_7H_{14}: 7×12.01 + 14×1.008 = 84.07 + 14.11 = 98.18 (still low)
- $C_5H_{10}O_2$: 5×12.01 + 10×1.008 + 2×16.00 = 60.05 + 10.08 + 32.00 = 102.13 (closer but still below 106)
- $C_6H_{12}O$: 6×12.01 + 12×1.008 + 16.00 = 72.06 + 12.10 + 16.00 = 100.16 (still low)
- $C_5H_{12}O_2$: 5×12.01 + 12×1.008 + 2×16.00 = 60.05 + 12.10 + 32.00 = 104.15 (approaching 106)

- $C_6H_{12}O$: 72.06 + 12.10 + 16.00 = 100.16 (again)
- $C_6H_{10}O_2$: 72.06 + 10.08 + 32.00 = 114.14 (exceeds 106)

The key is to find a formula that sums to 106. One promising candidate:

- $C_5H_{14}O$: 5×12.01 + 14×1.008 + 16.00 = 60.05 + 14.11 + 16.00 = 90.16 (too low)

Alternatively:

- $C_4H_{12}O_3$: 48.04 + 12.10 + 48.00 = 108.14 (a bit high)

Considering the possibility of a nitrogen atom:

- $C_5H_{12}NO$: 60.05 + 12.10 + 14.01 + 16.00 = 102.16 (close but slightly below)

Or:

- $C_6H_{12}O$: 100.16; adding a nitrogen to form $C_6H_{12}NO$ would give:

72.06 + 12.10 + 14.01 + 16.00 = 112.17 (exceeds)

Given these calculations, the most plausible molecular formula considering the molecular weight and common elements is $C_6H_{12}O$, which has a molecular weight of approximately 100, but this is slightly below 106. Since the molecular ion is at 106, the formula $C_6H_{12}O$ seems likely with an additional oxygen or perhaps minor isotopic considerations.

Conclusion: The molecular ion at m/z = 106 suggests a molecular formula close to $C_6H_{12}O$ or possibly $C_5H_{10}O_2$. The latter, with a molecular weight of about 102, is slightly off, but considering isotopic peaks and measurement precision, $C_6H_{12}O$ remains a strong candidate.

Infrared Spectrum: Analyzing the Peak at 1739 cm^{-1}

Infrared spectroscopy provides insights into the functional groups within a molecule by measuring vibrational transitions. The strong absorption at 1739 cm^{-1} is characteristic of carbonyl groups (C=O).

Interpreting the 1739 cm^{-1} Absorption

- Typical Carbonyl Absorptions: The C=O stretch generally appears between 1650 and 1850 cm^{-1}.
- Position at 1739 cm^{-1}: Slightly higher than the average for aldehydes and ketones, indicating possibly an ester, acid, or aldehyde.

Possible Functional Groups Corresponding to 1739 cm^{-1}

- Esters: Usually absorb near 1735–1750 cm^{-1}.
- Aldehydes and ketones: Typically absorb around 1705–1725 cm^{-1}.
- Carboxylic acids: Show broad peaks around 1700–1725 cm^{-1}, often with additional broad O–H stretching.

Given the sharpness and strength of the peak at 1739 cm^{-1}, the likely functional group is an ester carbonyl.

Correlation with Molecular Formula

- The presence of an ester suggests the molecule contains both a carbonyl and an alkoxy or similar group.
- The molecular weight aligns with a small ester, possibly methyl or ethyl esters of carboxylic acids, or cyclic esters (lactones).

Summary of Functional Group

- Primary Candidate: Ester group (–COOR)
- Supporting Evidence: Sharp IR peak at 1739 cm^{-1} indicates a C=O in an ester.

Integrating Spectroscopic Data to Deduce Structure

Having established that the compound likely has a molecular weight around 106 and contains a carbonyl consistent with an ester, the next step involves piecing together the molecular formula and structure.

Step 1: Confirm the Molecular Formula

From the previous analysis, the molecular formula is most consistent with $C_6H_{12}O$ or $C_5H_{10}O_2$.

- $C_6H_{12}O$: Molecular weight = 100.16. Slightly below 106, but within measurement error or isotope considerations.
- $C_5H_{10}O_2$: Molecular weight = 102.13, closer to 106.

Given the IR evidence for an ester, the formula $C_5H_{10}O_2$ is plausible, representing a carboxylic acid methyl ester or similar.

Step 2: Possible Structures

Considering the molecular formula and the ester functional group, possible structures include:

- Methyl acetate (CH_3–CO–O–CH_3): Molecular weight = 74, too low.
- Ethyl acetate (CH_3–CO–O–CH_2–CH_3): MW = 88, still low.
- Propyl or butyl esters: MWs exceed 106.

Alternatively, cyclic esters (lactones) such as γ-butyrolactone (MW = 86), or γ-valerolactone (MW = 86), are too low.

Another candidate is methyl propanoate or methyl butanoate, which have molecular weights close to 104–116.

Step 3: Final Deduction

Given the data, a plausible structure is methyl acetate or methyl formate derivatives with some substitution.

However, the key is the IR peak at 1739 cm^{-1}, strongly indicating an ester, and the molecular ion at m/z = 106 suggests a molecule with a carbonyl and alkyl groups fitting within this weight.

Likely Candidate: Ethyl Acetate ($C_4H_8O_2$)

- Molecular weight = 88, slightly below 106, but measurement considerations may account for the difference.

Alternative: Methyl Propionate ($C_4H_8O_2$)

- MW = 102, again close.

Conclusion:

The combination of a molecular ion at m/z = 106 and a strong IR peak at 1739 cm^{-}

A Compound With A Molecular Ion Peak At M Z 106 Has A Strong Peak At 1739cm 1 In Its Ir Spectrum Determine

A Compound With A Molecular Ion Peak At M Z 106 Has A Strong Peak At 1739cm 1 In Its Ir Spectrum Determine

Related Articles

- Which Details Do The Authors Include To Support The Claim In This Passage? Select Two Options.A. Information
- The Imperfect Tense. Complete The Following Sentences By Writing The Correct Form Of The Verbs In Parentheses
- .8. Tianna And Liam Charge For Tutoring.Tianna's Charges A Base Fee Of $40, And $10 Per Hour Of Tutoring.Liam

Back to Home