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Understanding the analytical techniques used in organic chemistry is essential for identifying and characterizing compounds. Among these techniques, mass spectrometry (MS) and infrared (IR) spectroscopy play pivotal roles. When combined, they offer comprehensive insights into the molecular structure, functional groups, and molecular weight of unknown compounds. This article delves into the significance of a mass spectrum showing a molecular ion at m/z = 113 and the characteristic features of its IR spectrum, providing a detailed guide for chemists and students alike.

Interpreting the Mass Spectrum: The Significance of M/z = 113

Mass spectrometry is a powerful analytical tool that measures the mass-to-charge ratio (m/z) of ionized molecules. The appearance of a molecular ion peak at m/z = 113 provides critical information about the molecular weight and possible structure of the compound.

Understanding the Molecular Ion Peak

The molecular ion, often denoted as $M^{+\bullet}$, represents the intact molecule that has been ionized but not fragmented. Its m/z value corresponds to the molecular weight of the compound, assuming it carries a single positive charge.

- Molecular Weight Determination: A peak at m/z = 113 indicates that the molecular weight of the compound is approximately 113 g/mol.
- Isotopic Considerations: The molecular ion can sometimes show isotopic patterns, especially if the molecule contains elements like Cl or Br. The absence of such patterns suggests a molecule primarily composed of elements like C, H, N, O, etc.

Possible Molecular Formulas Corresponding to M/z = 113

Based on common elemental compositions, several molecular formulas can correspond to a molecular weight of 113. Common possibilities include:

- C_9H_{13}
- C_8H_{17}
- $C_7H_{17}O$
- $C_6H_{13}NO$
- $C_5H_{11}N_2O$

Determining the exact formula requires further analysis, including degree of unsaturation, fragmentation patterns, and IR data.

Infrared (IR) Spectroscopy: Characteristic Features

IR spectroscopy provides information about the functional groups present in a molecule by measuring the absorption of infrared light at characteristic wavelengths. The IR spectrum of this compound exhibits characteristic peaks that help identify its functional groups.

Key IR Absorption Regions and Their Significance

The IR spectrum typically displays peaks in specific regions, each corresponding to particular bond vibrations:

Wavenumber Range (cm^{-1})	Functional Group / Vibration
3200–3600	O-H and N-H stretching vibrations
2800–3100	C-H stretching (aliphatic or aromatic)
1650–1750	C=O stretching (carbonyl groups)
1500–1600	C=C stretching (aromatic rings)
1000–1300	C-O stretching (ethers, esters)

Characteristic IR Peaks for This Compound

Based on typical spectral features:

- A broad peak around 3300 cm^{-1} suggests the presence of O-H or N-H groups. The broadness indicates hydrogen bonding, common in alcohols or amines.
- A sharp peak near 1700 cm^{-1} indicates the presence of a carbonyl group (C=O), suggesting ketones, aldehydes, carboxylic acids, or esters.
- Peaks between 2850–2950 cm^{-1} correspond to C-H stretching, confirming the presence of hydrocarbons.
- Additional peaks in the 1000–1300 cm^{-1} region point to C-O bonds, indicative of ethers, esters, or carboxylic acids.

Integrating Mass Spectrometry and IR Data for Structural Elucidation

Combining the insights from the mass spectrum and IR spectrum allows chemists to propose plausible structures for the compound.

Step-by-Step Approach

1. **Determine the Molecular Formula:** Use the molecular weight (113 g/mol) and elemental analysis to derive possible formulas.

2. **Identify Functional Groups:** Use IR peaks to identify key functional groups such as carbonyl, hydroxyl, amino, or ether groups.

3. **Analyze Fragmentation Patterns:** Examine MS fragmentation peaks to infer the presence of specific substructures.

4. **Propose Structures:** Based on the above data, suggest possible compounds that fit all spectral features.

Example Candidate Structures

Given the data, some plausible structures include:

- Acetaldehyde (C_2H_4O): Molecular weight of 44 g/mol, too low.
- Methyl acetate ($C_3H_6O_2$): Molecular weight of 74 g/mol, too low.
- Aromatic ketone, such as propiophenone ($C_9H_{10}O$): Molecular weight of 134 g/mol, slightly high.
- A primary candidate could be an organic compound like N-methylacetamide (C_3H_7NO) with molecular weight 73 g/mol, again too low.

Considering the molecular weight of 113 g/mol, a likely candidate is butanone (C_4H_8O) with a molecular weight of 72 g/mol, so perhaps a substituted derivative.

Alternatively, a compound like ethyl acetate ($C_4H_8O_2$) has a molecular weight of 88 g/mol, still lower.

Hence, the compound might be a heteroatom-containing molecule, such as an amide or ester with substituents increasing the molecular weight.

Practical Applications of Spectral Data in Organic Chemistry

Spectral analysis is an indispensable part of organic synthesis and research. The combined use of mass spectrometry and IR spectroscopy provides:

- Rapid identification: Quickly narrows down possible molecular structures.
- Structural confirmation: Validates the presence of functional groups and molecular weight.
- Purity assessment: Identifies impurities or by-products in samples.
- Mechanistic insights: Helps understand reaction pathways by analyzing intermediates.

Conclusion

The detection of a molecular ion at m/z = 113 in the mass spectrum indicates that the compound's molecular weight is approximately 113 g/mol. When complemented by characteristic IR spectral features—such as peaks indicative of carbonyl groups, hydroxyl or amino groups, and hydrocarbon stretches—these data collectively facilitate the identification and structural elucidation of the compound. While additional spectroscopic methods like NMR could further refine the structure, the combined mass and IR data already provide a robust foundation for understanding the compound's nature. Mastery of interpreting such spectral data is essential for chemists involved in organic synthesis, analytical chemistry, and related fields, enabling accurate characterization and advancing scientific knowledge in chemical research.

Frequently Asked Questions

What does a molecular ion at M/z = 113 indicate about the compound's molecular weight?

It indicates that the molecular weight of the compound is approximately 113 atomic mass units, representing the ionized molecular species in the mass spectrum.

What are common functional groups associated with IR spectra characteristic of compounds with a molecular ion at m/z 113?

Depending on the IR spectrum's features, characteristic groups could include aromatic rings, C-H stretches, or specific functional groups like esters or alcohols, but more details are needed for precise identification.

How can mass spectrometry help determine the molecular formula of this compound?

By analyzing the molecular ion peak at m/z 113 and considering isotopic patterns, fragmentation patterns, and exact mass, one can deduce the possible molecular formulas consistent with that molecular weight.

What typical fragmentation patterns might be observed in the mass spectrum of a compound with M/z = 113?

Common fragmentation may include loss of small neutral molecules (like water or methyl groups), ring cleavages if aromatic, or specific fragment ions that help infer the structure, depending on the compound's functional groups.

How does the IR spectrum assist in confirming the functional groups present in the compound?

IR spectroscopy reveals characteristic absorption bands corresponding to specific functional groups, such as O-H, N-H, C=O, or C-H stretches, helping to elucidate the compound's structure.

What additional analytical techniques could complement mass spectrometry and IR to identify this compound?

NMR spectroscopy (^{1}H and ^{13}C), UV-Vis spectroscopy, and chromatography techniques (like GC or HPLC) can provide further structural and purity information to confirm the compound's identity.

Based on the molecular ion at m/z 113 and IR data, what classes of

compounds are likely candidates?

Possible candidates include aromatic compounds like substituted benzene derivatives, small esters, or alkylbenzenes, but precise identification requires detailed IR and fragmentation analysis.

Additional Resources

The Mass Spectrum Of This Compound Shows A Molecular Ion At M/z = 113, The IR Spectrum Has Characteristic

In the realm of organic chemistry and analytical techniques, mass spectrometry (MS) and infrared (IR) spectroscopy remain two of the most powerful tools for elucidating molecular structures. When combined, these methods provide a comprehensive picture of a compound's molecular weight, structural features, and functional groups. Recently, a particular compound has garnered attention due to its distinctive spectral signatures: its mass spectrum reveals a molecular ion at m/z = 113, while its IR spectrum exhibits characteristic absorption bands. This article delves into the significance of these spectral features, exploring how they aid in identifying and confirming the compound's structure, and providing insights into the underlying chemistry.

Understanding the Mass Spectrum: Significance of the Molecular Ion at m/z = 113

The Basics of Mass Spectrometry

Mass spectrometry is an analytical technique used to determine the molecular weight and structural elements of a compound. The process involves ionizing molecules, separating the resulting ions based on their mass-to-charge ratio (m/z), and detecting these ions to generate a spectrum. The key features in a mass spectrum include the molecular ion peak (also called the parent ion), fragment peaks, and sometimes isotopic patterns.

The Molecular Ion Peak at m/z = 113

The observation of a molecular ion at m/z = 113 indicates that the molecular weight of the neutral compound is approximately 113 atomic mass units (amu). This peak is crucial because it confirms the molecular mass, setting the foundation for deducing the molecular formula.

- Significance: The molecular ion provides the molecular weight, which, combined with isotopic patterns and elemental composition considerations, guides the determination of the molecular formula.

- Isotopic Considerations: The presence of characteristic isotopic peaks (e.g., from ^13C, ^37Cl, or ^81Br if halogens are involved) can further refine the proposed formula.

Inferring the Molecular Formula

Given the molecular weight of 113, chemists employ various methods to propose potential formulas. For example:

- Common elements: Carbon (C), hydrogen (H), nitrogen (N), oxygen (O), halogens (Cl, Br).

- Sample calculations:
- $C8H13$: Molecular weight = $(8\times12.01) + (13\times1.008) \approx 96.08 + 13.104 \approx 109.18$ (too low)
- $C7H13N$: $\approx (7\times12.01) + (13\times1.008) + 14.01 \approx 84.07 + 13.104 + 14.01 \approx 111.18$ (close)
- $C9H13$: $\approx (9\times12.01) + (13\times1.008) \approx 108.09 + 13.104 \approx 121.19$ (too high)

A plausible molecular formula could be $C8H13NO$ (molecular weight $\approx$ 139), which is too high, or perhaps $C7H13NO$ ($\approx$ 113), fitting the observed m/z. Precise calculations and isotopic pattern analysis are critical here.

Interpreting the IR Spectrum: Characteristic Absorption Bands

The Role of IR Spectroscopy

Infrared spectroscopy provides information about the vibrational modes of bonds within a molecule. Different functional groups absorb IR radiation at characteristic wavenumbers, producing a spectrum that serves as a molecular fingerprint.

Key IR Absorptions in the Spectrum

The IR spectrum of the compound in question exhibits certain characteristic absorption bands, which suggest the presence of specific functional groups:

- O-H or N-H Stretch (around 3300-3500 cm^{-1}): If a broad, strong peak appears here, it indicates hydroxyl or amine groups.

- C-H Stretch (around 2800-3100 cm^{-1}): The presence of aliphatic or aromatic C-H bonds.

- C=O Stretch (around 1650-1750 cm^{-1}): A sharp peak here suggests a carbonyl group.

- C=C Stretch (around 1600-1680 cm^{-1}): Indicates aromatic or alkene functionalities.

- C-O or C-N Stretches (around 1000-1300 cm^{-1}): Suggests ethers, esters, or amines.

Deduction of Functional Groups

Suppose the spectrum shows:

- A moderate to broad peak at ~3400 cm^{-1}: indicative of N-H or O-H stretch.

- A sharp peak at ~1700 cm^{-1}: suggests a carbonyl group, possibly an aldehyde, ketone, or ester.

- Multiple peaks between 2850-3100 cm^{-1}: characteristic of C-H stretching in aliphatic or aromatic systems.

This combination points toward a molecule containing either an amine or hydroxyl group, along with a carbonyl functionality—common in compounds such as amides, esters, or aldehydes.

Integrating Mass Spectral and IR Data: Towards Structural Elucidation

Constructing the Structural Framework

By combining the molecular weight information with functional group clues:

- Molecular weight of 113 suggests a relatively small organic molecule.

- Presence of a carbonyl (from IR) indicates possible aldehyde, ketone, ester, or amide.

- N-H or O-H groups imply the molecule could be an amide, amine, alcohol, or acid derivative.

Possible Structural Classes

Given these clues, some candidate structures include:

- Amino acids or derivatives: e.g., amino acids with side chains fitting the molecular weight.

- Aromatic compounds with substituents: e.g., substituted benzene derivatives with functional groups.

- Small esters or aldehydes: e.g., acetaldehyde derivatives or methyl esters.

Narrowing Down the Options

Suppose the molecular formula is $C_8H_{13}NO$, aligning with the observed molecular weight. This formula suggests:

- A nitrogen atom (N) and oxygen atom (O) within the structure.

- Likely a molecule containing an amine or amide group, possibly attached to an alkyl chain or aromatic ring.

- The IR spectrum supporting the presence of an N-H stretch and a carbonyl group.

A representative candidate could be N-methylpiperidine, a cyclic amine with molecular weight 113, which exhibits IR bands characteristic of secondary amines and cyclic structures.

Confirming the Structure: Additional Techniques and Considerations

While MS and IR provide valuable clues, definitive structural confirmation often requires supplementary techniques:

- Nuclear Magnetic Resonance (NMR) Spectroscopy: Offers detailed information about the hydrogen and carbon skeleton.

- Elemental Analysis: Confirms the proposed molecular formula.

- Other Spectroscopic Methods: Such as UV-Vis or Raman spectroscopy.

- Crystallography: For unambiguous structural determination if suitable crystals can be obtained.

Practical Applications and Significance

Understanding the spectral features of this compound has broader implications:

- Pharmaceutical development: Identifying bioactive molecules with specific functional groups.

- Material science: Designing compounds with desired properties based on their structure.

- Environmental analysis: Detecting and characterizing pollutants or natural products.

The ability to interpret mass spectra and IR spectra efficiently enables chemists to rapidly identify unknown compounds, confirm synthetic products, and elucidate complex molecular architectures.

Conclusion

The combined analysis of mass spectrometry and infrared spectroscopy provides a powerful approach for characterizing organic compounds. In this case, the molecular ion at m/z = 113 indicates a small, likely organic molecule, while characteristic IR absorption bands suggest specific functional groups such as amines, carbonyls, or hydroxyls. By integrating these spectral insights, chemists can narrow down the structure, guiding further investigations with NMR and other techniques. Ultimately, these analytical tools serve as the backbone of molecular identification, advancing research across pharmaceuticals, materials, and environmental sciences.

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