What is Mass Spectrometry?

Worksheet

MS vaporizes and ionizes a sample, then uses electric/magnetic fields to separate ion fragments by m/z ratio, creating a mass spectrum that identifies the molecular ion and its fragments.

Questions

1. A mass spectrum of an organic compound shows m/z = 58 as the base peak. If the molecular ion is at m/z = 88, what neutral fragment was lost?

A) 12 (carbon)
B) 14 (CH)
C) 30 (CHO or NO)
D) 16 (oxygen)

2. Which would give the highest m/z peak in a mass spectrum?

A) A small fragment ion
B) The molecular ion (M) or a peak very close to it
C) A doubly charged ion
D) The base peak

3. Why do carboxylic acids often show a weak M peak?

A) They cannot be ionized
B) They easily lose -OH to form a stable acylium ion [RCO]
C) They have high molecular weight
D) Carboxylic acids do not fragment

4. In electron impact (EI) ionization, what removes an electron from the sample?

A) A laser
B) High-energy electrons
C) An electric field
D) A photon

5. A mass spectrum of ethanol (CHOH, MW 46) shows peaks at m/z = 46, 31, and 29. Explain each peak.

6. A mass spectrum shows m/z = 100 as the base peak (most intense). What does this suggest?

7. Benzoic acid (CHO, MW 122) has a very weak M peak. Why?

8. Define: What is the m/z ratio?

9. Define: What is the molecular ion (M)?

10. Define: What is the base peak?

Answer Key

1. C) 30 (CHO or NO) - 88 58 = 30, indicating loss of a 30 u fragment (likely CHO from an ester or NO from a nitro compound).

2. B) The molecular ion (M) or a peak very close to it - The highest m/z molecular weight (M). Fragments have lower m/z. Multiply charged ions have lower m/z for the same mass.

3. B) They easily lose -OH to form a stable acylium ion [RCO] - Carboxylic acids readily lose the -OH group, forming a stable [RCO] acylium ion, making M less prominent.

4. B) High-energy electrons - EI uses high-energy electrons (typically 70 eV) to remove an electron from the molecule, creating the radical cation M.

5. m/z = 46: Molecular ion M (CHOH) - not always prominent m/z = 31: [CHOH] loss of CH (46 15 = 31) m/z = 29: [CHO] or [HCO] from further fragmentation These fragments are characteristic of alcohols.

6. The base peak is the most stable cation formed from the sample. If m/z = 100 is very stable, it likely results from loss of a small, stable neutral molecule. This could be M HO, M CH, or another characteristic loss. The m/z value provides clues about the molecular structure.

7. Carboxylic acids easily lose -OH (17 mass units) forming m/z = 105 [CHCO] This acylium ion is very stable and becomes the base peak. Weak M = easy fragmentation to a stable, charged fragment. This is a characteristic pattern for carboxylic acids and esters.

8. Mass-to-charge ratio - mass of an ion divided by its charge. For singly charged ions, m/z = mass.

9. The radical cation formed by removing one electron from the neutral molecule - represents the molecular weight.

10. The most intense peak in a mass spectrum - usually corresponds to the most stable fragment ion.