Mass Spectrometry Chemistry Questions with Solutions

Q1. The mass analyser is similar to which of the following in optical spectrometer?

(a) Monochromator
(b) Detector
(c) Sample
(d) Source

Answer: (a), The mass analyser is similar to a monochromator.

Q2. What are the main criteria for which a mass spectrometer is used?

(a) To find the composition of the sample
(b) To find the relative mass of atoms
(c) To find the concentration of elements in the sample
(d) To find the properties of the sample

Answer: (b), Mass spectrometry is primarily used to find the relative mass of atoms.

Q3. Mass spectrometry was discovered by whom?

(a) Walter Kaufmann
(b) J. J Thomson
(c) Francis Aston
(d) Ernest O. Lawrence

Answer: (b), Mass spectrometry was discovered by J. J Thomson.

Q4. A mass spectrometer separates ions based on which the following factors?

(a) Mass
(b) Charge
(c) Molecular Weight
(d) Mass to charge ratio

Answer: (d), A mass spectrometer separates ions based on mass to charge ratio.

Q5. Can two molecules fragment in the same manner?

(a) True
(b) False
(c) Sometimes
(d) Can't be determined.

Answer: (a), No two molecules can fragment in the same manner

Q6. What are the uses of mass spectrometry?

Answer: Mass spectrometry is primarily used

- To measure the relative molar mass with high precision and deduce a compound's molecular formula.
- To detect the site of fragmentation in a molecule which enables the detection of recognisable groupings in the molecule.
- To identify an unknown compound by comparing its mass spectrum with the digitalised mass spectra usually available in university libraries.

Q7. What does a mass spectrometer do after ionisation and fragmentation to provide a mass spectrum?
Answer: The spectrometer sorts out all the cations (including the radical cations) according to their mass/charge (m/z or m/e) values and records them as line signals along the abscissa. At the same time, the instrument records their relative abundances as signal heights plotted as intensities along the ordinate. The mass spectrometer does not detect the radicals.

Q8. Why can the m/z values be taken as the molar mass of the cation?
Answer: We can take m/z values as the molar mass of the cation because the charge on the cation (z) is +1, making m/z = m.

Q9. Why do several signals appear in a typical spectrum?
Answer: Several signals appear in a typical spectrum because parent hydrocarbon can fragment in different ways, and each cationic fragment can further fragment to give smaller cations.

Q10. If an RS^+ contains only carbon, hydrogen and oxygen, will its m/z value be odd or even?
Answer: If an RS^+ contains only carbon, hydrogen and oxygen, its m/z value is even because the presence of oxygen in a formula does not change the carbon to hydrogen ratio. Since the mass of oxygen is even, the mass of RS^+ with carbon, hydrogen and oxygen must be even.

Q11. Why do we use less than 1 mg of the parent compound in the vapour state for analysis?
Answer: We use less than 1 mg of the parent compound in the vapour state for analysis to prevent collisions and reactions between fragments. A combination of fragments might lead to ions with larger masses than the parent cation, making it impossible to determine the molar mass. Fragmentation patterns useful in structure determination would become confusing if taken in large quantities.

Q12. Give the molecular formula of hydrocarbon cation with an m/z value of 91.
Answer: To calculate the molecular formula of hydrocarbon cation with an m/z value of 91, we will divide the given value by 12 to get the number of carbon atoms. The remainder of the mass is due to hydrogens. Hence the molecular formula of the parent hydrocarbon cation is $C_7H_7^+$.

Q13. Give the molecular formula of hydrocarbon cation with an m/z value of 51.

Answer: To calculate the molecular formula of hydrocarbon cation with an m/z value of 51, we will divide the given value by 12 to get the number of carbon atoms. The remainder of the mass is due to hydrogens. Hence the molecular formula of the parent hydrocarbon cation is $C_4H_3^+$.

Q14. Give the molecular formula of hydrocarbon cation with an m/z value of 29.
Answer: To calculate the molecular formula of hydrocarbon cation with an m/z value of 29, we will divide the given value by 12 to get the number of carbon atoms. The remainder of the mass is due to hydrogens. Hence the molecular formula of the parent hydrocarbon cation is $C_2H_5^+$.

Q15. Give the structure of compound $C_{10}H_{12}O$, whose mass spectrum shows m / z values of 15,43, 57, 91, 105 and 148.
Answer: A peak at m / z = 15 suggests a CH_3 group. As 43 - 15 = 28, the mass of CO, the m/z value of 43, may be due to an acetyl group, CH_3CO group in the compound. The highest peak gives the molar mass. Cleaving an acetyl group (m / z = 43) from the 148 gives 105, an observed peak. Next below 105 is 91, a difference of 14; this suggests a CH_2 group attached to CH_3CO. So far, we have CH_3COCH_2 adding up to 57, leaving 148 - 57 = 91. This peak is likely to be $[C_7H_7]^+$, whose precursor is the stable benzyl cation, $C_6H_5CH_2^+$. Piecing together all this information, the structure $CH_3COCH_2CH_2C_6H_5$.

Practise Questions on Mass Spectrometry

Q1. Give a combination of carbon, nitrogen and hydrogen to account for the m/z value of 29?

Answer: If one nitrogen is present, subtracting the mass of nitrogen (14) leaves a mass of 15, suitable for one carbon and three hydrogens. Thus, the formula of the compound is CH_3N^+.

Q2. Give a combination of carbon, nitrogen and hydrogen to account for the m/z value of 57?

Answer: If one nitrogen is present, subtracting the mass of nitrogen (14) leaves a mass of 43, suitable for three carbon and seven hydrogens. Thus, the formula of the compound is $C_3H_7N^+$.
If two nitrogen is present, subtracting the mass of nitrogen (28) leaves a mass of 29, suitable for two carbon and five hydrogens. Thus, the formula of the compound is $C_2H_5N_2^+$.
If three nitrogen is present, subtracting the mass of nitrogen (42) leaves a mass of 15, suitable for one carbon and three hydrogens. Thus, the formula of the compound is $CH_3N_3^+$.

Q3. Why can an atom with an m/z value of 31 not be $C_2H_7^+$?

Answer: An atom with an m/z value of 31 is not $C_2H_7^+$ because the largest number of hydrogen for two carbon atoms is six.

Q4. Give a combination of atoms to account for the m/z value of 31?

Answer: A combination of atoms to account for the m/z value of 31 can be with nitrogen and oxygen. If one nitrogen is present, subtracting the mass of nitrogen (14) leaves a mass of 17, suitable for one carbon and five hydrogens. Thus, the formula of the compound is CH_5N^+.
If one oxygen atom is present, subtracting the mass of oxygen (16) leaves a mass of 15, suitable for one carbon and three hydrogens. Thus, the formula of the compound is CH_3O^+.

Q5. Give the molecular formula of hydrocarbon cation with an m/z value of 28.

Answer: To calculate the molecular formula of hydrocarbon cation with an m/z value of 28, we will divide the given value by 12 to get the number of carbon atoms. The remainder of the mass is due to hydrogens. Hence the molecular formula of the parent hydrocarbon cation is $C_2H_4^{2+}$.