Exercise walk-through

22.2
Mass spectrometry

A-Level Chemistry

What we will cover

1. Infrared spectroscopy
2. Mass spectrometry
3. Molecular ion & fragments
4. [M+1] & [M+2] peaks

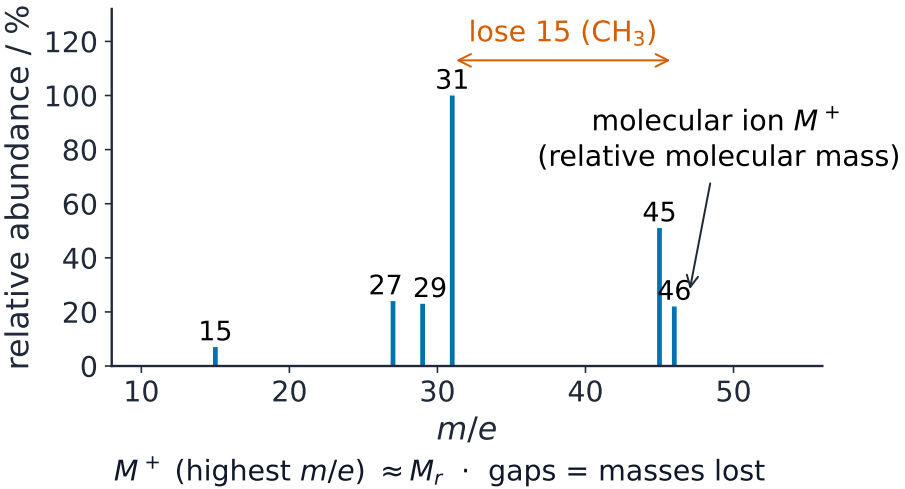


sorts ions by mass

Mass spectrometry

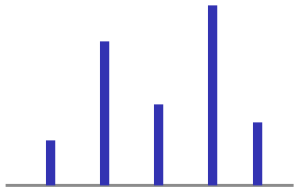
Mass spectrometry sorts ions by **mass-to-charge ratio** (m/e).

> The highest-m/e peak is the **molecular ion** M^+ ($= M_r$); the gaps between peaks give the masses of the lost **fragments** (loss of 15 = CH_3).



Check yourself

1. Which bond absorbs around 1700 cm^{-1}?
2. What does the highest-m/e peak give?
3. A loss of 15 means which fragment was lost?
4. An [M+2] peak in a 1:1 ratio shows which halogen?



Answers **1.** C=O **2.** the relative molecular mass **3.** CH_3 **4.** bromine

Exercises 2.1·2.2

2.1 State what the molecular ion peak (highest m/e) tells you about a compound. [1]

2.2 A mass spectrum shows a peak at M and another of nearly equal height at M+2. What element is present? [1]

Exercises 2.1·2.2

2.1 State what the molecular ion peak (highest m/e) tells you about a compound. [1]

2.1

- its molecular mass / M_r (the mass of the whole molecule)

2.2 A mass spectrum shows a peak at M and another of nearly equal height at M+2. What element is present? [1]

2.2

- bromine (Br) – the ^{79}Br/^{81}Br ratio is about 1:1

Exercises 3.1–3.2

3.1 Chlorine has isotopes $^{35}\mathrm{Cl}$ (75%) and $^{37}\mathrm{Cl}$ (25%). Its relative atomic mass is: [1]

- ☐ **A** 35.0
- **B** 35.5
- **C** 36.0
- **D** 37.0

3.2 Loss of a fragment of mass 15 from a molecular ion suggests the loss of: [1]

- ☐ **A** OH
- **B** $\mathrm{CH_3}$
- **C** $\mathrm{C_2H_5}$
- **D** Cl

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3.1 B

- $A_r = \dfrac{(35 \times 75) + (37 \times 25)}{100} = 35.5$

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- ☐ **A** OH
- **B** CH_3
- **C** C_2H_5
- **D** Cl

3.2 B

- A loss of 15 is a CH_3 group

Exercise 3.3 (a)

3.3 A compound has a molecular ion peak M^+ at m/e = 88 (abundance 100) and an [M+1] peak (abundance 4.4).

(a) Use $n = \dfrac{100 \times \text{abundance of } [M+1]}{1.1 \times \text{abundance of } M^+}$ to find the number of carbon atoms. [2]

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(a)

- $n = \dfrac{100 \times 4.4}{1.1 \times 100} = 4$

Exercise 3.3 (b)

3.3 A compound has a molecular ion peak M^+ at m/e = 88 (abundance 100) and an [M+1] peak (abundance 4.4).

(b) The compound is a carboxylic acid of M_r 88. Suggest its molecular formula. [1]

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(b)

- $C_4H_8O_2$ (e.g. butanoic acid)

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3.4

- bromine; the two peaks two apart in a ~1:1 ratio match the ^{79}Br and ^{81}Br isotopes