

Exercise walk-through

Mass spectrometry ■ 22.2

eXercise

You must be able to

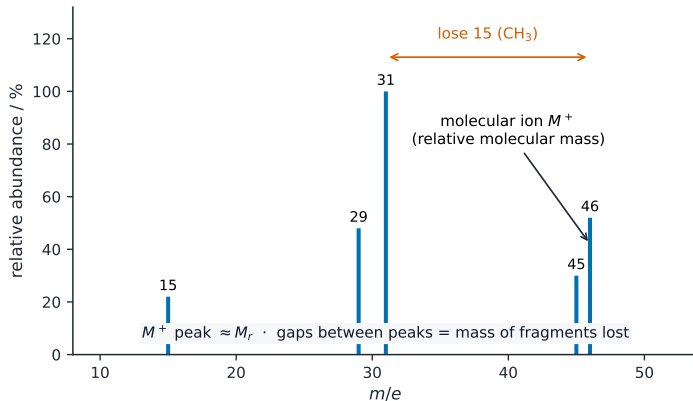
- calculate relative atomic mass from isotopic abundances or a mass spectrum
- deduce molecular mass from the molecular ion peak and identify fragments
- use the $[M+1]$ peak to find the number of carbons, and $[M+2]$ for Cl/Br

Method — Relative atomic mass and the molecular ion

*The peaks are at different m/e values; the **molecular ion** M (highest m/e) gives the M_r*

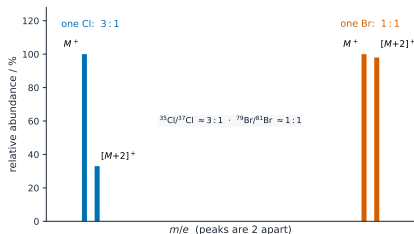
$$A_r = \frac{\sum(\text{isotope mass} \times \text{abundance})}{\sum \text{abundance}}$$

Method — Relative atomic mass and the molecular ion



A mass spectrum with peaks at different m/e values, the molecular ion at the highest m/e

Method — Fragmentation, $[M+1]$ and $[M+2]$



- **fragments:** the molecule breaks into smaller ions; the mass lost identifies the group (e.g. loss of 15 = CH).
- **$[M+1]$ carbon count:**
$$n = \frac{100 \times \text{abundance of } [M+1]}{1.1 \times \text{abundance of } M^+}.$$
- **$[M+2]$:** a peak two higher $\rightarrow$ Cl (3:1) or Br (1:1).

Practice 2.1 ■ 1 mark

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

Solution 2.1

Method: Relative atomic mass and the molecular ion

Worked steps

its molecular mass / M_r (the mass of the whole molecule) **B1**.

Practice 2.2 ■ 1 mark

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

Solution 2.2

Method: Fragmentation, $[M+1]$ and $[M+2]$

Worked steps

bromine (Br) — the Br/ ^{79}Br ratio is about 1:1 **B1**.

Exam-style 3.1 ■ 1 mark

Chlorine has isotopes ^{35}Cl (75%) and ^{37}Cl (25%). Its relative atomic mass is:

A 35.0

B 35.5

C 36.0

D 37.0

Solution 3.1

Method: Relative atomic mass and the molecular ion

A 35.0

B 35.5



C 36.0

D 37.0

Worked steps

$$\text{B. } A_r = \frac{(35 \times 75) + (37 \times 25)}{100} = 35.5.$$

Exam-style 3.2 ■ 1 mark

Loss of a fragment of mass 15 from a molecular ion suggests the loss of:

A OH

B CH

C C H

D Cl

Solution 3.2

A OH

B CH 

C C H

D Cl

Worked steps

B. A loss of 15 is a CH group.

Exam-style 3.3 ■ 2 marks

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

- (a) Use $n = \frac{100 \times \text{abundance of } [M+1]}{1.1 \times \text{abundance of } M^+}$ to find the number of carbon atoms.
- (b) The compound is a carboxylic acid of M_r 88. Suggest its molecular formula.

Solution 3.3

Method: Fragmentation, $[M+1]$ and $[M+2]$

Worked steps

$$(a) \ n = \frac{100 \times 4.4}{1.1 \times 100} = 4 \quad \text{M1 A1}.$$

(b) $\text{C}_4\text{H}_8\text{O}_2$ (e.g. butanoic acid) B1.

Exam-style 3.4 ■ 2 marks

A mass spectrum has peaks at $m/e = 78$ and 80 in a 1:1 ratio. State, with a reason, which halogen is present.

Solution 3.4

Method: Relative atomic mass and the molecular ion

Worked steps

bromine **M1**; the two peaks two apart in a $\sim 1:1$ ratio match the Br and ^{81}Br isotopes **A1**.