A-LEVEL CHEMISTRY • EXERCISE SHEET

22.2 Mass spectrometry

Name: _____ Class: _____ Date: _____ **Total: 9 marks**

KEY WORDS molecular ion 分子离子 • molecular ion peak 分子离子峰 • relative atomic mass 相对原子质量 • isotopic abundance 同位素丰度 • mass spectrometry 质谱

Objective

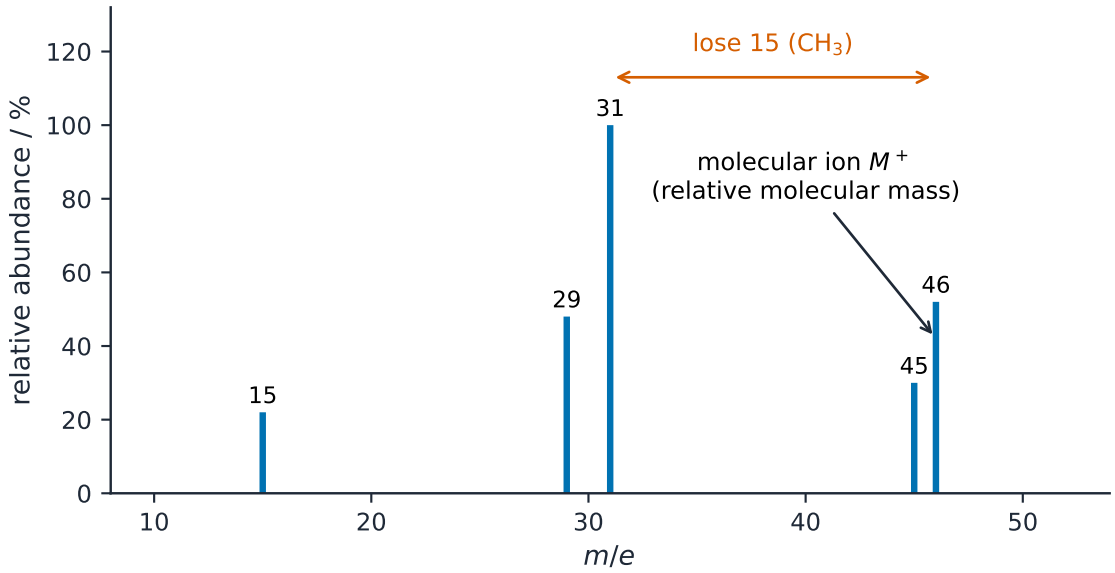
Build the skills to answer exam questions on **mass spectrometry** 质谱 — the **molecular ion** 分子离子, **fragmentation** 碎裂, the **[M+1]** carbon count, and the **[M+2]** halogen test.

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

1 Worked examples

■ Relative atomic mass and the molecular ion

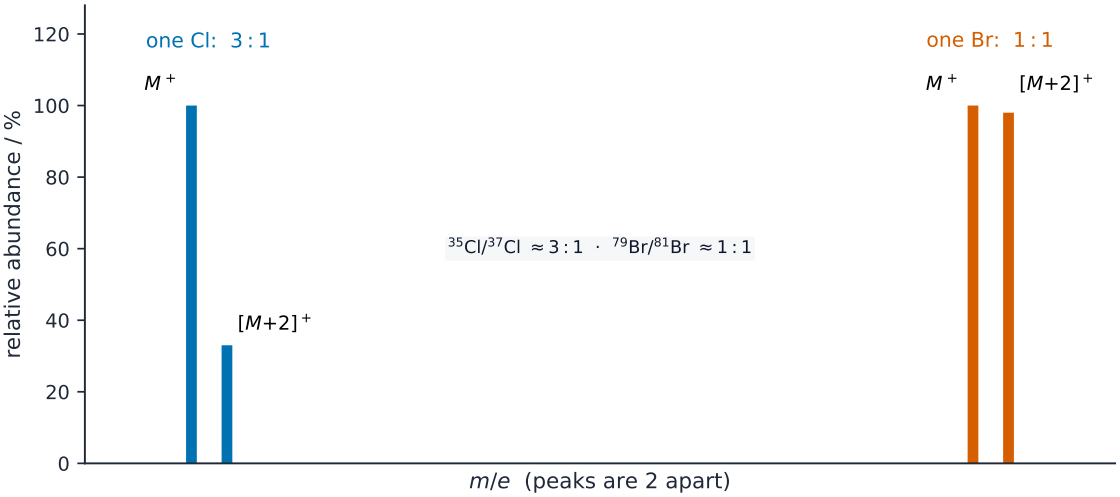


M^+ peak $\approx M_r$ · gaps between peaks = mass of fragments lost

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

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

Fragmentation, [M+1] and [M+2]



A small [M+1] peak comes from ^{13}C; an [M+2] peak shows a Cl or Br atom

- **fragments:** the molecule breaks into smaller ions; the mass lost identifies the group (e.g. loss of 15 = CH_3).
- **[M+1] carbon count:** $n = \dfrac{100 \times \text{abundance of } [M+1]}{1.1 \times \text{abundance of } M^+}$.
- **[M+2]:** a peak two higher → Cl (3:1) or Br (1:1).

2 Practice

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]

3 Exam-style questions

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

A B
C D

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 B
C D

A OH
B CH_3
C C_2H_5
D Cl

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]

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

3.4 A mass spectrum has peaks at m/e = 78 and 80 in a 1:1 ratio. State, with a reason, which halogen is present. [2]