

22 Analysis (spectroscopy) – Part 2

Name: _____ Class: _____ Date: _____

Vocabulary

Write each word three times.

English	Write it 3 times (English)
Mass spectrometry	_____
mass-to-charge ratio	_____
molecular ion peak	_____
fragmentation	_____
fragment	_____

Recall

Mass spectrometry is another analysis tool. It turns a molecule into ions and sorts them by their **mass-to-charge ratio** (m/e).

- The spectrum is a set of peaks at different m/e values.
- The tallest-mass peak tells you the molecule's mass.

New ideas

Read these first, then do the Practice.

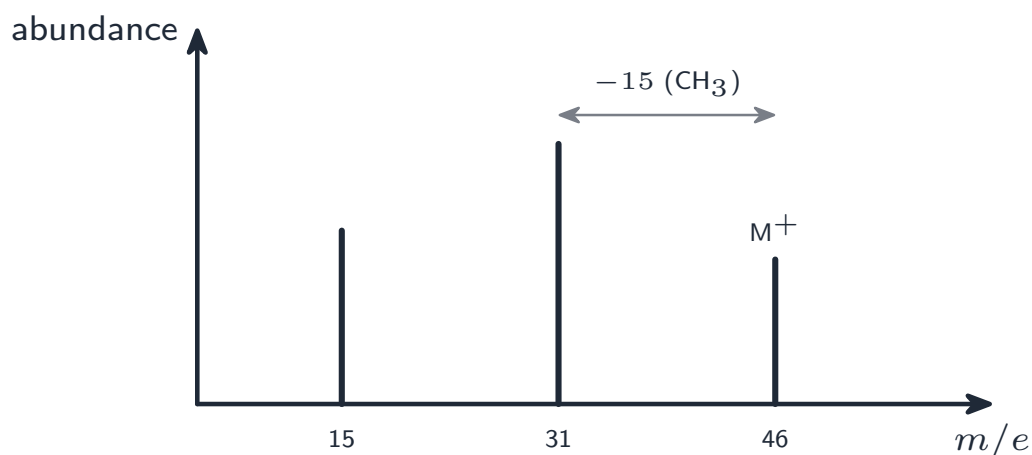
■ 1 The molecular ion peak

The peak at the **highest** m/e is the **molecular ion peak** (M^+). It gives the **relative molecular mass** (M_r) of the whole molecule.

■ 2 Fragmentation

The molecule also breaks into smaller pieces – **fragmentation**. The **gap** between two peaks gives the mass of the piece lost, so you can suggest each **fragment**:

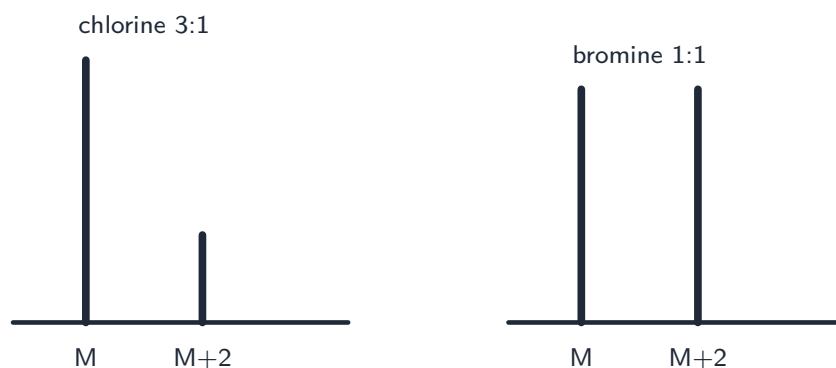
- a loss of **15** = a CH_3 group.
- a loss of **29** = CHO or C_2H_5 .



■ 3 The $[M+2]$ peak shows a halogen

An $[M+2]$ peak two mass units above M^+ shows chlorine or bromine:

- one **chlorine** gives an $[M+2]$ about **one third** the height of M^+ (a **3:1** ratio).
- one **bromine** gives an $[M+2]$ about the **same** height as M^+ (a **1:1** ratio).



Watch out: the molecular ion (highest m/e) gives M_r ; the *gap* between peaks gives the mass *lost* (the fragment), not the fragment's own peak. An $[M+2]$ peak means chlorine (3:1) or bromine (1:1).

Practice

Try these in order.

22.1 What does the molecular ion peak (M^+) tell you? [1]

22.2 Where on the spectrum is the molecular ion peak found? [1]

22.3 A spectrum shows peaks at $m/e = 46$ and 31. What fragment was lost, and what is it? [2]

22.4 An $[M+2]$ peak is the same height as the M^+ peak. Which halogen is present? [1]

22.5 What peak ratio shows that one chlorine atom is present? [1]

22.6 Challenge. A spectrum has its molecular ion at $m/e = 78$ and an $[M+2]$ peak at $m/e = 80$ of about the *same* height. Suggest the halogen present, and explain. [2]
