Topic 7: Modern Analytical Techniques I

Edexcel A Level Chemistry • Paper 1 (9CH0/01)

7.1

Be able to use mass spectrometry data to: (i) determine Mr from the molecular ion peak, (ii) suggest structures from fragmentation patterns.

(i) Molecular ion peak (M^+): the peak with the highest m/z value (ignoring M+1) gives the relative molecular mass directly. The M+1 peak is caused by ^{13}C isotopes and is not the molecular ion.

(ii) Fragmentation: the molecular ion breaks into smaller pieces in the mass spectrometer. Each fragment peak represents a positively charged fragment lost from M^+. Look at the difference between M^+ and each fragment peak to identify the group lost.

Common fragment losses:

–15 = loss of CH_3 (methyl group)

–17 = loss of OH (hydroxyl)

–28 = loss of CO (carbonyl)

–29 = loss of CHO (aldehyde group) or C_2H_5 (ethyl group)

–31 = loss of CH_2OH (from primary alcohol)

–45 = loss of OC_2H_5 (ethoxy group, from ethyl ester)

Base peak = the most abundant fragment (tallest peak in the spectrum). It is not necessarily the molecular ion.

© Chemistry with Chloe | chemistrywithchloe.com
For personal educational use only. Not for redistribution.

7.2

Be able to use IR spectra to deduce functional groups and predict absorptions.

Infrared (IR) spectroscopy identifies functional groups by the bonds present in a molecule. Each bond absorbs IR radiation at a characteristic wavenumber (cm^{-1}). Absorptions are shown as dips/troughs on an IR spectrum.

Key IR absorptions to know:

- O–H (alcohol): broad absorption, ~3230–3550 cm^{-1}
- O–H (carboxylic acid): very broad, ~2500–3300 cm^{-1} (overlaps with C–H)
- C=O (aldehyde, ketone, acid, ester): strong, sharp, ~1680–1750 cm^{-1}
- C=C (alkene): ~1620–1680 cm^{-1}
- C–H (alkane): ~2850–2960 cm^{-1}
- N–H (amine): ~3300–3500 cm^{-1}

Carboxylic acid identification: look for BOTH a broad O–H absorption AND a strong C=O absorption together.

Fingerprint region: below ~1500 cm^{-1}. This region is unique to each compound and is used to confirm identity by comparison with a reference spectrum. It is too complex to interpret bond by bond.

Always use data provided in the exam. You do not need to memorise exact wavenumbers but must know the approximate ranges.

Analysis of Some Inorganic and Organic Unknowns

ABOUT THESE NOTES

Notes written by Chloe Archard (MSc Biochemistry, Oxford-trained chemist, 20+ years teaching experience at top UK independent schools). For 1-1 tuition, revision courses, and more free resources: chemistrywithchloe.com

© Chemistry with Chloe | chemistrywithchloe.com
For personal educational use only. Not for redistribution.