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IB DIPLOMA CHEMISTRY · FIRST ASSESSMENT 2025

Structure 3.2
Mass Spectrometry & IR Spectroscopy

Booklet 7 (HL) · Understandings 3.2.8 – 3.2.9

How the fragments of a molecule in a mass spectrometer reveal its structure, and how the bonds in a molecule announce themselves by absorbing infrared radiation

Complete revision notes, practice spectra & memory points · Higher Level

How the level tags work in this booklet

HL **Everything in this booklet is Higher Level only.** Understandings 3.2.8 (mass spectrometry of organic compounds) and 3.2.9 (infrared spectroscopy) are not assessed at Standard Level.

SL + HL Short reminder panels recap the SL material the HL work builds on: the mass spectrometer (Structure 1.2), the electromagnetic spectrum (Structure 1.3), bond polarity (Structure 2.2) and functional groups (Booklet 4).

Inside this booklet

1. What the syllabus actually asks of you
2. 3.2.8 — The mass spectrometer and fragmentation
3. 3.2.8 — Interpreting mass spectra
4. 3.2.9 — Infrared radiation and bond vibrations
5. 3.2.9 — IR-active molecules and greenhouse gases
6. 3.2.9 — Interpreting IR spectra
7. Key points to memorise
8. Check yourself
9. Answers

1 What the syllabus actually asks of you

Booklets 4 to 6 showed how to draw, classify and name an organic molecule when you already know its structure. In the laboratory the problem usually runs the other way: you have a colourless liquid and need to find out what it is. Chemists solve this with instruments. A **mass spectrometer** weighs the molecule and the pieces it breaks into; an **infrared spectrometer** shows which bonds, and so which functional groups, are present. Together with ^{1}H NMR (the next booklet) they can identify almost any small organic compound from a few milligrams of sample.

Understanding	What it says	What you must be able to do	Level
3.2.8 Mass spectrometry	Mass spectrometry (MS) of organic compounds can cause fragmentation of molecules.	Deduce information about the structural features of a compound from specific MS fragmentation patterns. Include reference to the **molecular ion**. Data on specific MS fragments are provided in the data booklet.	HL
3.2.9 Infrared spectroscopy	Infrared (IR) spectra can be used to identify the type of bond present in a molecule.	Interpret the **functional group region** of an IR spectrum, using a table of characteristic frequencies (wavenumber / cm^{-1}). Include reference to the absorption of IR radiation by **greenhouse gases**. Data for interpreting IR spectra are given in the data booklet.	HL

Linking questions and connections for 3.2.8 – 3.2.9

- **Structure 1.2:** the mass spectrometer and the mass spectra of elements (isotopes). → section 2.1
- **Structure 1.3:** the electromagnetic spectrum, $c = f\lambda$ and $E = hf$. → section 4.1
- **Structure 2.2:** what features of a molecule determine whether it is IR active or not? → section 5.1
- **Reactivity 1.3:** what properties of a greenhouse gas determine its 'global warming potential'? → section 5.3
- **Booklet 4 (3.2.2):** functional groups are what the IR spectrum detects. → section 6
- **Next booklet (HL 3.2.10 – 3.2.12):** ^{1}H NMR, and combining MS, IR and NMR to identify a compound. → section 6.6 gives a preview.

What the data booklet gives you — and what it does not

- **Section 22** lists the **masses of neutral fragments lost** from the molecular ion (15, 17, 18, 28, 29, 31, 45). It does **not** list the masses of the fragment **ions** themselves (such as 43 for CH_3CO^+), so you must work those out from relative atomic masses.
- **Section 20** gives the IR **wavenumber ranges and intensities** of the bonds you need. You are not expected to memorize them, but you must know how to use them, and the typical shapes of the signals.
- The data booklet also gives c, h and L for the wavenumber and energy calculations. It does not tell you which molecules are IR active or how to reason from a spectrum: that is the skill this booklet practises.

2 Structure 3.2.8 — The mass spectrometer and fragmentation HL

2.1 Reminder: how a mass spectrometer works SL + HL

In Structure 1.2 the mass spectrometer was used to find the masses and abundances of the isotopes of an element. Exactly the same instrument can 'weigh' a molecule. The sample is vaporized, ionized, accelerated and separated according to the **mass-to-charge ratio**, m/z, of each ion. Almost all the ions formed carry a 1+ charge, so m/z is simply the mass of the ion.



Figure 1 — The stages in a mass spectrometer. Only ions are accelerated, deflected and detected; neutral particles are not affected by electric or magnetic fields.

2.2 The molecular ion

In the ionization chamber, a high-energy electron from an electron gun strikes a molecule and knocks out one of its electrons:

$$M(g) + e^- \rightarrow M^+(g) + 2e^-$$

Definitions to learn

- The **molecular ion** (or parent ion), M^+, is the ion formed when a molecule loses one electron but otherwise remains unchanged. Its m/z value is equal to the **relative molecular mass**, M_r.
- The molecular ion peak is normally the peak with the **highest m/z** in the spectrum (ignoring the very small M+1 peak caused by ^{13}C atoms, section 3.5).
- The **base peak** is the tallest peak in the spectrum. It is given a relative abundance of 100% and every other peak is measured against it. It belongs to the most abundant, usually the most stable, ion, and it is often **not** the molecular ion.

Knowing M_r is already useful: combined with an empirical formula from combustion analysis (Structure 1.4), it gives the molecular formula.

2.3 Fragmentation

The ionizing collision transfers so much energy that many molecular ions do not survive the journey: a bond breaks and the ion splits into two pieces. One piece keeps the positive charge and is detected; the other is a neutral **radical** (shown with a dot, •) or molecule, and is **not** detected.

$$M^+ \rightarrow X^+ + Y^\bullet \quad \text{e.g.} \quad CH_3CH_2OH^+ \rightarrow CH_2OH^+ \ (m/z = 31) + {}^\bullet CH_3 \ (\text{mass 15, not detected})$$

The same bond can break either way round, and the charge stays on whichever piece forms the more stable cation. Breaking the C–C bond in ethanol could give CH_3^+ ($m/z = 15$) or CH_2OH^+ ($m/z = 31$); the oxygen helps to stabilize the positive charge, so the 31 peak is far larger. The set of peaks a compound gives, its **fragmentation pattern**, is reproducible and characteristic of that compound, like a fingerprint. Two isomers have the same molecular ion but different fragmentation patterns, because their atoms are joined differently.

Fragments to recognise

Data booklet Section 22 gives the mass **lost**. The ions themselves you work out by adding up relative atomic masses (C 12, H 1, O 16). These are the ones that appear most often:

Mass lost (Section 22)	Neutral fragment lost		*m/z* of ion	Common fragment ion
15	$^{\bullet}CH_3$		15	CH_3^+
17	$^{\bullet}OH$		29	$C_2H_5^+$ or CHO^+
18	H_2O		31	CH_2OH^+ (primary alcohols) or OCH_3^+
28	$CH_2{=}CH_2$ or CO		43	$C_3H_7^+$ or CH_3CO^+
29	$^{\bullet}CH_2CH_3$ or $^{\bullet}CHO$		45	$COOH^+$ or CH_3CHOH^+
31	$^{\bullet}OCH_3$		57	$C_4H_9^+$ or $C_2H_5CO^+$
45	$^{\bullet}COOH$		77	$C_6H_5^+$ (a phenyl group)

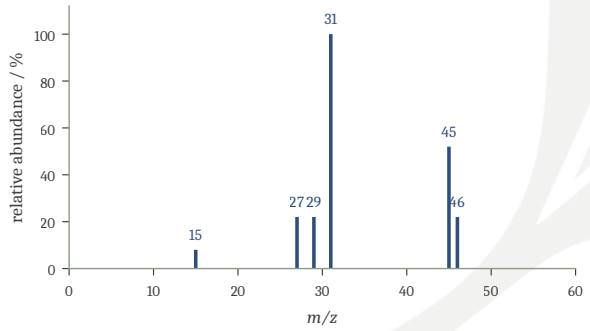
Some masses have two possible identities (43 can be $C_3H_7^+$ or CH_3CO^+; 28 can be lost as C_2H_4 or CO). Use the other evidence to decide.

3 Structure 3.2.8 — Interpreting mass spectra HL

Method — interpreting a mass spectrum

1. Find the **molecular ion** (highest *m/z*): this is M_r. With an empirical formula, deduce the molecular formula.
2. Work out the **mass lost** for the large peaks near M^+: M − 15 (lost CH_3), M − 17 (OH), M − 29 (C_2H_5 or CHO), M − 45 (COOH) and so on, using data booklet Section 22.
3. Identify the **ions** responsible for the main low-*m/z* peaks (15, 29, 31, 43, 45, 57…), especially the base peak.
4. Propose a structure that would produce these fragments by breaking single bonds, and check that it gives no fragments that are **missing** from the spectrum. Always write the formula of an ion with its + charge.

3.1 Worked example — ethanol



m/z	Ion	Explanation
46	$CH_3CH_2OH^+$	molecular ion, M_r = 46
45	$CH_3CH_2O^+$	M − 1: loss of H
31	CH_2OH^+	M − 15: loss of $^{\bullet}CH_3$; base peak
29	$C_2H_5^+$	M − 17: loss of $^{\bullet}OH$
15	CH_3^+	C–C breaks, charge on CH_3

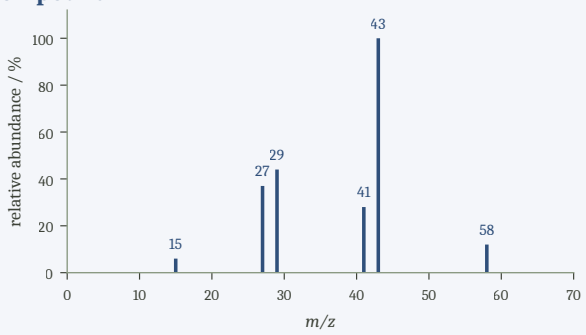
Figure 2 — A simplified mass spectrum of ethanol, C_2H_5OH. The base peak at 31 comes from breaking the C–C bond next to the oxygen, which is typical of primary alcohols. (The peak at 27, $C_2H_3^+$, forms when $C_2H_5^+$ loses H_2.)

3.2 Worked example — telling chain isomers apart

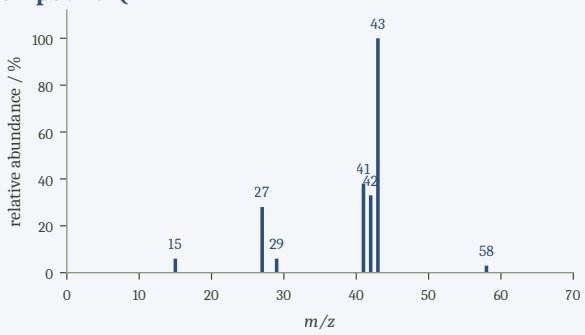
Worked example 2 — a hydrocarbon with empirical formula C_2H_5

Two hydrocarbons with the empirical formula C_2H_5 give the spectra below. Deduce the molecular formula, and identify each compound.

Compound P



Compound Q

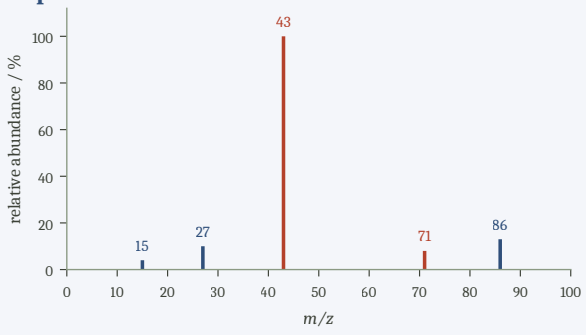


- Both molecular ions are at $m/z = 58$. C_2H_5 has a mass of 29, so $n = 58 \div 29 = 2$: the molecular formula is $\mathbf{C_4H_{10}}$. The two possibilities are butane and 2-methylpropane (Booklet 5).
- Both show a base peak at 43, $C_3H_7^+$ (M − 15, loss of CH_3), which either isomer can form.
- P has a large peak at **29**, $C_2H_5^+$. Splitting butane, $CH_3CH_2–CH_2CH_3$, down the middle gives two C_2H_5 pieces. 2-Methylpropane, $CH(CH_3)_3$, has no CH_2CH_3 group, so it can only give a tiny 29 peak.
- So P is **butane** and Q is **2-methylpropane**. The weaker molecular ion of Q is also typical: branched molecular ions fragment more easily.

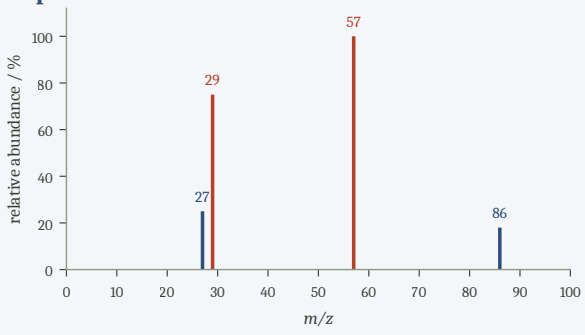
Worked example 3 — two ketones with the formula $C_5H_{10}O$

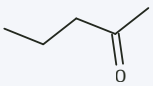
Pentan-2-one and pentan-3-one ($C_5H_{10}O$, $M_r = 86$) give the spectra below. Which is which?

Compound R

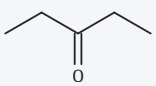


Compound S





pentan-2-one

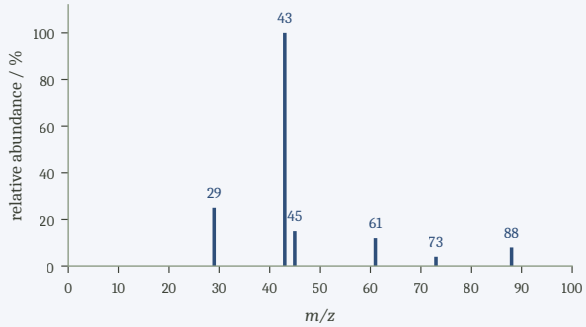


pentan-3-one

- Ketones break most easily at the bonds either side of the C=O. Pentan-3-one, $CH_3CH_2COCH_2CH_3$, is symmetrical: breaking either bond gives $C_2H_5CO^+$ ($m/z = 57$) and $C_2H_5^+$ (29). So **S is pentan-3-one**.
- Pentan-2-one, $CH_3COCH_2CH_2CH_3$, breaks to give CH_3CO^+ (43) or $C_3H_7CO^+$ (71, M − 15). So **R is pentan-2-one**. It has no 57 peak, because it has no $C_2H_5–C=O$ unit.

3.3 Worked example — empirical formula to structure

Worked example 4 — a compound with empirical formula C_2H_4O



A neutral compound with the empirical formula C_2H_4O gives this spectrum. It does not react with sodium carbonate (so it is not an acid). Deduce its structure.

1. Molecular ion at 88. C_2H_4O = 44, so n = 2: $\mathbf{C_4H_8O_2}$. This fits $C_nH_{2n}O_2$: a carboxylic acid or an ester. It is not an acid, so it is an **ester**.
2. Base peak 43 = CH_3CO^+: there is a CH_3–C=O unit, so the acid part is ethanoate.
3. 88 − 43 = 45 = OC_2H_5: the alcohol part is ethyl. The peak at 45 is $OC_2H_5^+$ and the peak at 29 is $C_2H_5^+$.
4. The compound is **ethyl ethanoate**, $CH_3COOCH_2CH_3$. (Its isomer methyl propanoate, $CH_3CH_2COOCH_3$, would instead show $C_2H_5CO^+$ at 57, formed by loss of OCH_3, M − 31.)

This spectrum also shows peaks at 61 and 73 (M − 15). You do not have to explain every peak; explain the important ones and make sure your structure does not predict large peaks that are absent.

3.4 Patterns worth knowing

Class	Typical fragments
alkanes	a series of peaks 14 apart (15, 29, 43, 57…): $C_nH_{2n+1}^+$; molecular ion weaker for branched alkanes
primary alcohols, RCH_2OH	31, CH_2OH^+; M − 18 (loss of water) is common
secondary alcohols, $RCH(OH)CH_3$	45, CH_3CHOH^+
aldehydes, RCHO	29, CHO^+; M − 1 and M − 29
methyl ketones, CH_3COR	43, CH_3CO^+, usually the base peak; M − 15
carboxylic acids, RCOOH	M − 17 (OH), M − 45 (COOH) and 45, $COOH^+$
esters, RCOOR′	RCO^+ (43 for ethanoates); M − 31 for methyl esters (OCH_3)
benzene compounds	77, $C_6H_5^+$

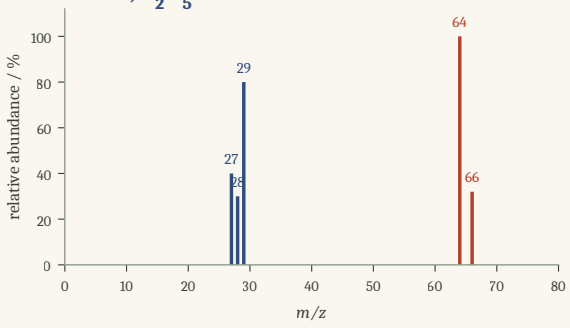
3.5 Isotope peaks

Going further (linked to Structure 1.2) — M+1, M+2 and the halogens

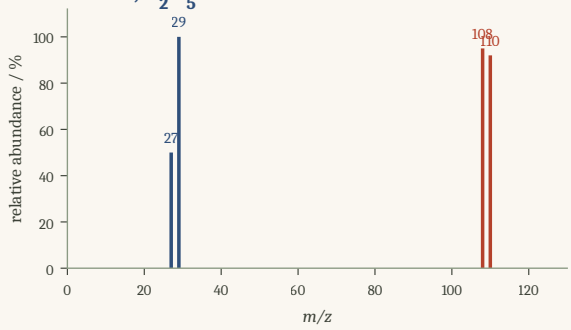
About 1.1% of carbon atoms are ^{13}C, so organic compounds show a small **M+1** peak one unit above the molecular ion; the more carbon atoms, the bigger it is. Chlorine and bromine have two common isotopes, so their compounds show two molecular ion peaks two units apart:

- chlorine: ^{35}Cl : $^{37}Cl \approx 3 : 1$, so a compound with one Cl atom shows M and M+2 peaks in a **3 : 1** ratio (chloroethane: 64 and 66);
- bromine: ^{79}Br : $^{81}Br \approx 1 : 1$, so one Br atom gives M and M+2 peaks of **equal height** (bromoethane: 108 and 110).

chloroethane, C_2H_5Cl



bromoethane, C_2H_5Br



Isotope patterns are not named in 3.2.8, but they appear in data-based questions and they give away a halogen instantly.

Model answer: "The mass spectrum of propan-1-ol shows a molecular ion peak at m/z = 60 and a base peak at m/z = 31. Identify the species responsible for each peak." (2 marks)

m/z = 60: $CH_3CH_2CH_2OH^+$, the molecular ion **[1]**. m/z = 31: CH_2OH^+, formed by loss of $^{\bullet}C_2H_5$ (mass 29) **[1]**. (Both formulas need the + charge.)

Examiner traps in mass spectrometry

- Every species you identify from a peak must be written as an **ion**, with its + charge: CH_3CO^+, not CH_3CO. Missing charges lose marks.
- The peak is caused by the fragment that is **detected** (the ion); the mass in data booklet Section 22 is the fragment **lost** (neutral). Do not confuse 'a peak at 15' (CH_3^+ detected) with 'M − 15' (CH_3 lost).
- The base peak is the tallest peak; the molecular ion is the one with the highest m/z. They are usually different.
- A peak at 43 does not prove a ketone: $C_3H_7^+$ also has m/z = 43. Use the molecular formula and the other peaks.
- Mass spectrometry gives the molecular formula and structural **clues**; it rarely proves a structure on its own. Combine it with IR (and, at HL, NMR).

Practice A **Name the fragment ions**

For each compound, give the formula (with its charge) of the ion responsible for each peak listed, and say which bond broke or which fragment was lost.

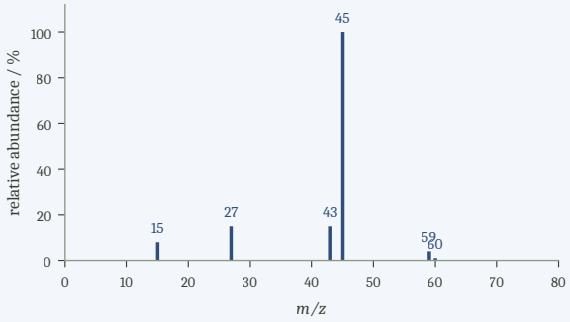
	Compound	Peaks to explain (m/z)
(a)	$CH_3CH_2CH_2CH_3$	15, 29, 43
(b)	CH_3COCH_3	15, 43
(c)	CH_3CH_2CHO	29, 57
(d)	CH_3COOH	15, 43, 45
(e)	CH_3CH_2OH	29, 31, 45
(f)	$CH_3CH(OH)CH_3$	45, 59
(g)	$C_6H_5CH_3$	77, 91
(h)	$CH_3CH_2COOCH_3$	29, 57, 59

Practice B **Identify the compound from its mass spectrum**

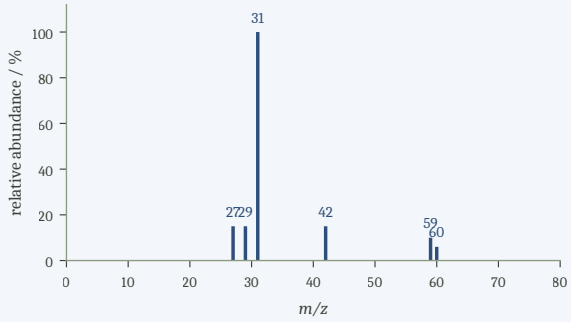
Each pair of compounds below are isomers. Use the spectra to decide which compound is which, and explain your choice by identifying key fragment ions.

(a) propan-1-ol, $CH_3CH_2CH_2OH$, and propan-2-ol, $CH_3CH(OH)CH_3$

Spectrum 1

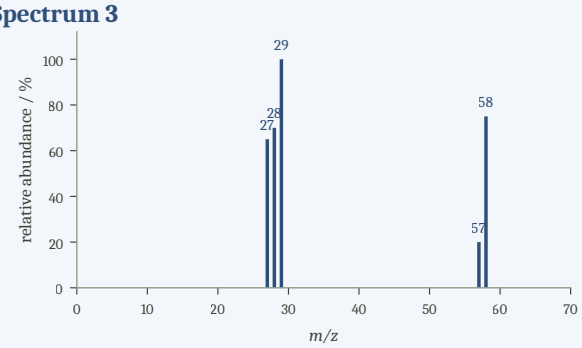


Spectrum 2

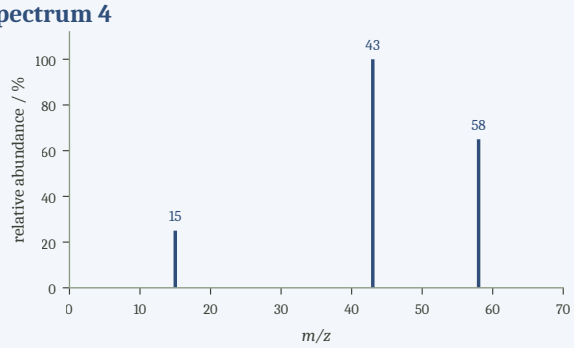


(b) propanal, CH_3CH_2CHO, and propanone, CH_3COCH_3

Spectrum 3

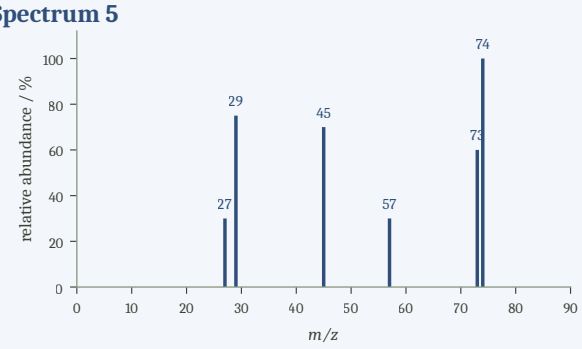


Spectrum 4

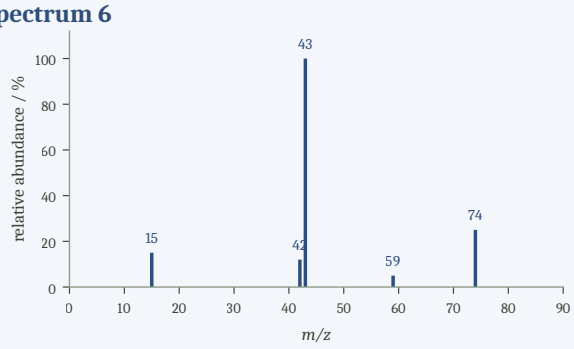


(c) methyl ethanoate, CH_3COOCH_3, and propanoic acid, CH_3CH_2COOH

Spectrum 5



Spectrum 6



Practice C **Molecular formulas and halogens**

Answer each part.

1. A compound with the empirical formula CH_2 has a molecular ion at $m/z = 84$. Deduce its molecular formula and suggest two possible classes of compound.
2. A compound with the empirical formula C_3H_6O has a molecular ion at 116. Deduce the molecular formula.
3. The molecular ion region of a halogenoalkane shows peaks at 78 and 80 in the ratio 3 : 1. Suggest its formula and explain the two peaks.
4. A compound shows molecular ion peaks at 122 and 124 of equal height and a large peak at 43. Suggest its structure.
5. Why is there no peak at $m/z = 17$ in the spectrum of ethanol, even though ethanol can lose an OH group?
6. 2,2-Dimethylpropane, $C(CH_3)_4$, shows almost no molecular ion at 72 but a base peak at 57. Explain.

4 Structure 3.2.9 — Infrared radiation and bond vibrations HL

4.1 Reminder: the electromagnetic spectrum SL + HL

Electromagnetic radiation carries energy and information. Each region of the spectrum interacts with molecules in a different way, and each gives a different kind of spectroscopy (Structure 1.3). The frequency f, wavelength λ and photon energy E are linked by $\boldsymbol{c = f\lambda}$ and $\boldsymbol{E = hf}$.

Region	Typical wavelength / m	What it does to molecules	Technique
radio waves	10^0 – 10^2	flips the spin of certain nuclei (^{1}H) in a magnetic field	NMR (next booklet)
microwaves	10^{-2}	increases rotational energy	microwave spectroscopy; ovens
infrared	10^{-6} – 10^{-4}	makes bonds **vibrate** more strongly: stretch and bend	**IR spectroscopy**
visible, UV	10^{-7} – 10^{-8}	excites electrons to higher energy levels	UV–visible spectroscopy
X-rays	10^{-10}	diffracted by the regular arrays of atoms in crystals	X-ray crystallography

4.2 Wavenumber

Definition and equations

IR spectroscopists describe radiation by its **wavenumber**, the number of waves in 1 cm, measured in cm^{-1}:

$$\text{wavenumber (cm}^{-1}\text{)} = 1 \div \text{wavelength (cm)}$$

Wavenumber is proportional to frequency and to photon energy: a **higher wavenumber means higher frequency, higher energy and shorter wavelength**. IR spectra run from about 4000 cm^{-1} (λ = 2.5 µm) down to about 500 cm^{-1} (λ = 20 µm).

Worked example 5 — converting between wavelength, wavenumber, frequency and energy

The C=O bond in propanone absorbs at 1715 cm^{-1}. Calculate (a) the wavelength, (b) the frequency and (c) the energy absorbed per mole of photons.

- (a) $\lambda = 1 \div 1715\ cm^{-1} = 5.83 \times 10^{-4}$ cm = **5.83×10^{-6} m** (5.83 µm).
- (b) $f = c/\lambda = 3.00 \times 10^{8} \div 5.83 \times 10^{-6}$ = **$5.15 \times 10^{13}\ s^{-1}$**.
- (c) $E = hf = 6.63 \times 10^{-34} \times 5.15 \times 10^{13} = 3.41 \times 10^{-20}$ J per photon; $\times 6.02 \times 10^{23} = 2.05 \times 10^{4}$ J mol^{-1} = **20.5 kJ mol^{-1}**.

Compare this with a C=O bond enthalpy of about 800 kJ mol^{-1}: IR radiation makes bonds vibrate, it does not break them.

4.3 Bonds behave like springs

A covalent bond can be modelled as two masses joined by a spring. It vibrates at a natural frequency, and it absorbs IR radiation of exactly that frequency, which makes it vibrate with a larger amplitude. Like a spring, the natural frequency depends on two things:

- **Bond strength** (the stiffness of the spring): stronger bonds vibrate at higher frequency. So C≡C (2100–2260) > C=C (1620–1680) > C–C, and C=O (1700–1750) > C–O (1050–1410).
- **Masses of the atoms**: lighter atoms vibrate at higher frequency. Bonds to hydrogen therefore absorb at the highest wavenumbers (O–H, N–H, C–H, all above 2500 cm^{-1}), and C–I (490–620) absorbs below C–Cl (600–800).

In a polyatomic molecule the whole molecule vibrates, in several distinct ways called **vibrational modes**: **stretching** (bond lengths change) and **bending** (bond angles change). Bending generally needs less energy than stretching, so bends absorb at lower wavenumbers.

Nature of Science — the limits of the spring model

The mass-on-a-spring picture is borrowed from everyday experience and it predicts the trends well, which is what makes it useful. But it is a simplification: real bonds are not perfect springs, and it is the molecule as a whole, not one isolated bond, that vibrates. Models in science are judged by how well they explain and predict, not by whether they are the 'real thing'.

5 Structure 3.2.9 — IR-active molecules and greenhouse gases HL

5.1 Which vibrations absorb IR radiation?

Key idea

A vibration absorbs IR radiation only if it causes a **change in the dipole moment** of the molecule. The oscillating electric field of the radiation can only 'push' on a vibration in which the separation of partial charges changes. Such a vibration is **IR active**; one that leaves the dipole moment unchanged is **IR inactive**.

- **Diatomic molecules** can only stretch. HCl, HBr and CO are polar, so stretching changes the dipole: they are IR active. Non-polar **N_2, O_2, H_2 and Cl_2** stay non-polar however they stretch: they are IR inactive. This is why the two main gases of the atmosphere are not greenhouse gases.
- The more polar the bond, the bigger the change in dipole and the **more intense** the absorption: that is why C=O and O–H give strong signals while C=C gives a weak one.

- A molecule does not need a permanent dipole to be IR active: CO_2 and CH_4 are non-polar overall, but some of their vibrations create a temporary dipole.

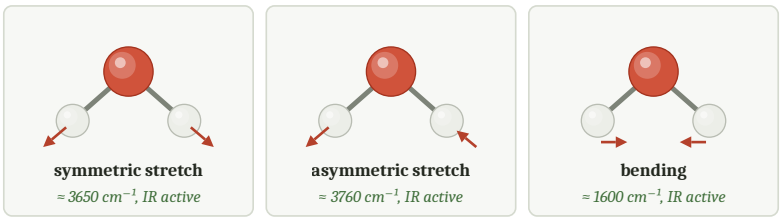


Figure 3 — The three vibrational modes of water. Each changes the dipole moment of the bent molecule, so all three are IR active.

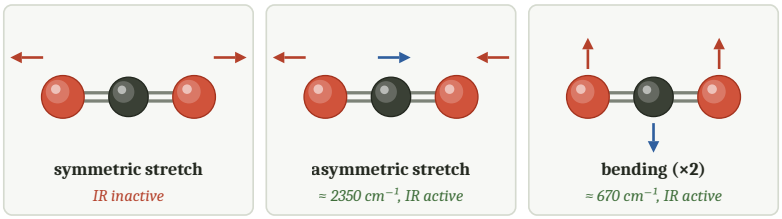


Figure 4 — The vibrational modes of carbon dioxide. In the symmetric stretch both C=O dipoles change equally and in opposite directions, so the molecule stays non-polar: IR inactive. The asymmetric stretch and the bends (one in the plane of the page, one perpendicular to it) create a temporary dipole: IR active.

Model answer: "Explain why carbon dioxide absorbs infrared radiation but nitrogen does not." (3 marks)

A vibration absorbs IR radiation only if it changes the dipole moment of the molecule **[1]**. The N≡N bond is non-polar and stretching it leaves the molecule non-polar, so N_2 is IR inactive **[1]**. In CO_2 the asymmetric stretch and the bending vibrations produce a temporary dipole (the C=O dipoles no longer cancel), so CO_2 absorbs **[1]**.

5.2 The greenhouse effect

Most of the Sun's energy reaches the Earth as visible and ultraviolet radiation, which passes through the atmosphere and warms the surface. The warm surface radiates energy back out as **longer-wavelength infrared radiation**. Greenhouse gases absorb some of this IR radiation, because it has the right frequencies to make their bonds vibrate, and then re-emit it in all directions, partly back towards the Earth. This keeps the lower atmosphere warmer than it would otherwise be.

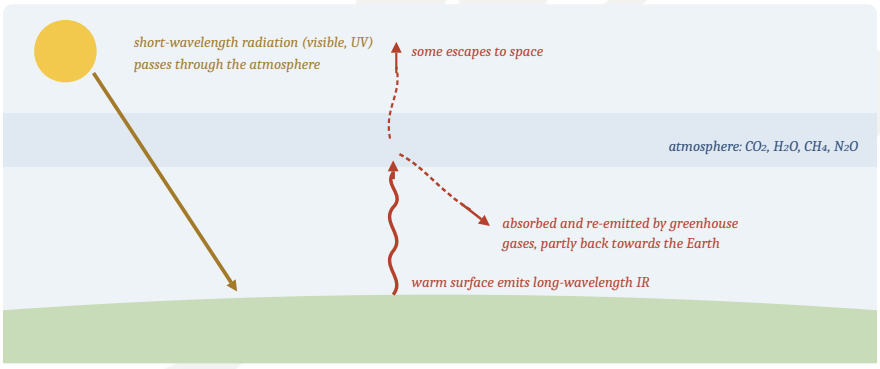


Figure 5 — The greenhouse effect. Without it the Earth's average surface temperature would be about −18 °C instead of about 15 °C; increasing the concentrations of greenhouse gases enhances it.

5.3 Global warming potential

Different greenhouse gases are not equally harmful. Their **global warming potential (GWP)** compares the energy absorbed by 1 tonne of the gas with that absorbed by 1 tonne of CO_2 over the same period (usually 100 years). It depends on:

- how strongly each molecule **absorbs IR radiation** (how many IR-active vibrations it has, at which wavelengths, and how large the dipole change is), and
- its **atmospheric lifetime**: how long it stays in the atmosphere before natural processes remove it.

Greenhouse gas	Formula	GWP (100 years)	Notes
carbon dioxide	CO_2	1	reference gas; by far the largest total effect because of its abundance
methane	CH_4	28	from agriculture, landfill and natural gas leaks
dinitrogen oxide (nitrous oxide)	N_2O	265	from fertilizers
HFC-134a	CH_2FCF_3	1300	refrigerant; not ozone-depleting, but now being phased out
CFC-13	$CClF_3$	13 900	refrigerant banned under the Montreal Protocol

GWP values from the IPCC Fifth Assessment Report (100-year horizon). Water vapour is the most abundant greenhouse gas, but its concentration is controlled by temperature rather than directly by emissions.

Examiner traps in IR activity and greenhouse gases

- The condition is a **change in dipole moment during the vibration**, not 'the molecule is polar'. CO_2 and CH_4 are non-polar but IR active.
- Greenhouse gases absorb the **long-wavelength IR** radiated by the Earth, not the incoming visible light from the Sun.
- IR radiation makes bonds **vibrate** (stretch or bend); it does not break them.
- Higher wavenumber = higher frequency = higher energy = **shorter** wavelength.

6 Structure 3.2.9 — Interpreting IR spectra HL

6.1 What an IR spectrum shows

In an IR spectrometer, IR radiation over a range of wavenumbers passes through the sample, and the detector measures how much is transmitted at each wavenumber. The spectrum plots **% transmittance** against **wavenumber**. Note two conventions that catch people out: the wavenumber axis runs **from high to low** (4000 cm^{-1} on the left), and absorptions point **downwards** as troughs from a baseline near 100%. Some instruments also change the scale of the axis at 2000 cm^{-1}.

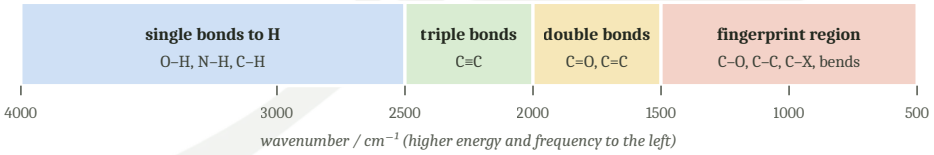


Figure 6 — The regions of an IR spectrum. Above 1500 cm^{-1} lies the **functional group region**, where individual bonds give recognisable absorptions. Below 1500 cm^{-1} lies the **fingerprint region**.

6.2 The data booklet table

Bond	Found in	Wavenumber / cm^{-1}	Intensity and shape
C–O	alcohols, esters, ethers	1050–1410	strong
C=C	alkenes	1620–1680	medium–weak; multiple bands
C=O	aldehydes, ketones, carboxylic acids, esters	1700–1750	**strong, sharp**
C≡C	alkynes	2100–2260	variable
O–H	carboxylic acids (hydrogen bonded)	2500–3000	**strong, very broad**
C–H	alkanes, alkenes, arenes	2850–3090	strong
O–H	alcohols and phenols (hydrogen bonded)	3200–3600	**strong, broad**
N–H	primary amines	3300–3500	medium; two bands

Selected rows of data booklet Section 20, which also lists C–F, C–Cl, C–Br and C–I absorptions in the fingerprint region. Always use the data booklet in the exam rather than memorized values.

Recognising the key signals by shape

- **O–H in alcohols**: a broad, rounded, strong trough around 3200–3600 cm^{-1}. Hydrogen bonding between molecules gives the O–H bonds a spread of slightly different strengths, which broadens the absorption and shifts it to lower wavenumber.
- **O–H in carboxylic acids**: an even broader trough from about 2500 to 3300 cm^{-1}, with the C–H absorptions sitting on top of it like a jagged edge.
- **C=O**: usually the deepest, sharpest trough in the spectrum, near 1700–1750 cm^{-1}. Very easy to spot.
- **C–H**: present in almost every organic compound around 2850–3090 cm^{-1}, so it rarely tells you much.
- **N–H** in a primary amine: two narrower, medium troughs at 3300–3500 cm^{-1}.

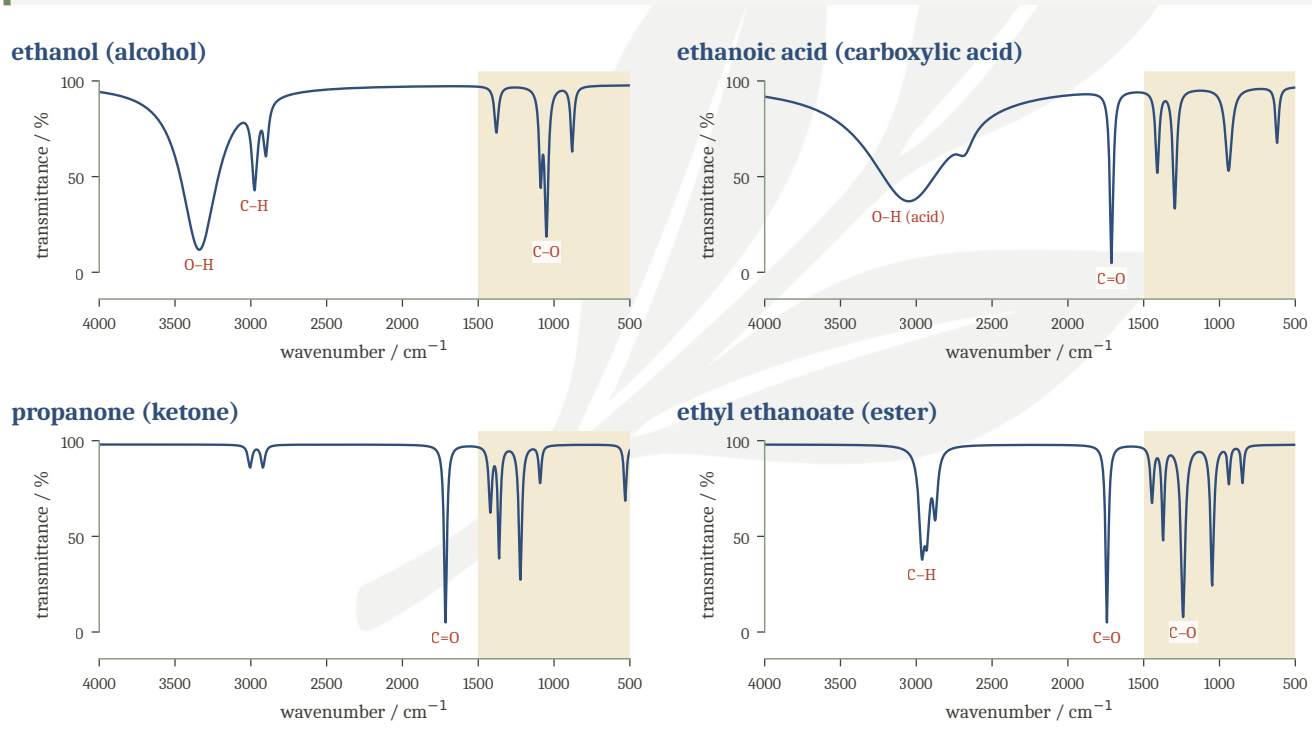


Figure 7 — Simplified IR spectra of four classes. The fingerprint region is shaded. Compare the two kinds of O–H, and notice that a C=O on its own cannot tell a ketone, an aldehyde, an acid and an ester apart: look at what else is there.

6.3 The fingerprint region

Below 1500 cm^{-1} there are many overlapping absorptions from C–C, C–O and C–X stretches and from bending vibrations of the whole molecule. Individual bonds are hard to assign here, but the overall pattern is unique to each compound. Matching it against a database of known spectra can **identify a specific compound**, and comparing a sample with a pure standard shows whether it is **pure**: any extra troughs come from an impurity. Forensic scientists use this to identify drugs, paints and fibres. The IB guide asks you to interpret the functional group region only.

6.4 Method

Method — interpreting an IR spectrum

1. Look first at **1700–1750**: a strong sharp trough means C=O (aldehyde, ketone, acid or ester).
2. Look at **2500–3600**: a broad trough at 3200–3600 means O–H in an alcohol; a very broad trough at 2500–3000 overlapping the C–H means O–H in an acid. A C=O **and** a very broad O–H together mean **carboxylic acid**.
3. C=O with a strong C–O (1050–1410) but no O–H suggests an **ester**; C=O with neither suggests an aldehyde or ketone.
4. Check for C=C (1620–1680, weak), C≡C (2100–2260) and N–H (3300–3500, two bands).
5. Use the **absence** of absorptions as evidence too: 'no broad absorption at 3200–3600, so no O–H'.
6. Always quote the bond **and** the wavenumber or range you used.

Worked example 6 — two isomers of $C_3H_6O_2$

Compounds A and B both have the formula $C_3H_6O_2$. Their IR spectra show:

	Absorptions / cm^{-1}
A	very broad 2500–3300; strong, sharp 1715; 1240
B	strong, sharp 1745; strong 1200 and 1050; nothing above 3100

- A: the very broad band at 2500–3300 is O–H in a carboxylic acid and 1715 is C=O. A is a carboxylic acid: **propanoic acid**, CH_3CH_2COOH.
- B: C=O at 1745 and C–O at 1050–1410, but no O–H. B is an ester: **methyl ethanoate**, CH_3COOCH_3, or **ethyl methanoate**, $HCOOCH_2CH_3$. IR alone cannot decide between them; the mass spectrum (or NMR) would.

Worked example 7 — following a reaction with IR

Propan-1-ol is heated under reflux with acidified potassium dichromate(VI). How would the IR spectrum show that the product is propanoic acid rather than unreacted alcohol? (Oxidation: Reactivity 3.2.)

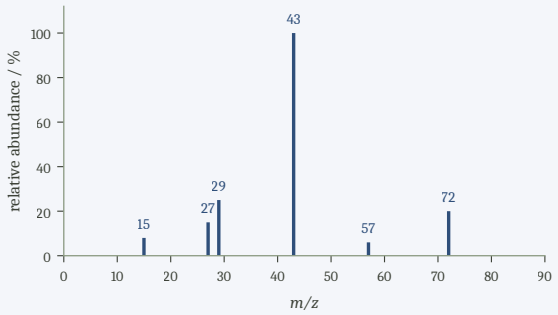
- Propan-1-ol: broad O–H at 3200–3600, C–O at about 1050, **no** C=O.
- Propanoic acid: a strong C=O at 1700–1750 **appears**, and the O–H absorption becomes the very broad acid band at 2500–3000.
- If the product were the aldehyde propanal (from distillation instead of reflux), there would be a C=O but **no** O–H absorption at all.

6.5 Breath testing

Roadside breath tests once relied on the colour change of orange dichromate(VI) to green chromium(III) when it oxidizes ethanol. Modern evidential instruments, called intoximeters, pass IR radiation through the driver's breath and measure the absorbance near 2900 cm^{-1}, due to the **C–H** bonds in ethanol. The amount absorbed is proportional to the concentration of ethanol (water vapour in breath does not absorb at this wavenumber, because it has no C–H bonds).

6.6 Putting MS and IR together

Worked example 8 — a preview of combined analysis (HL 3.2.12)



A compound contains 66.7% C, 11.1% H and 22.2% O by mass. Its IR spectrum shows a strong, sharp absorption at 1715 cm^{-1} and none between 3200 and 3600 cm^{-1}. Its mass spectrum is shown. Identify it.

1. Empirical formula: C 66.7/12.01 = 5.55; H 11.1/1.01 = 11.0; O 22.2/16.00 = 1.39; ratio 4 : 8 : 1, so C_4H_8O (72). M^+ = 72, so the molecular formula is C_4H_8O.
2. IR: C=O at 1715, no O–H: an aldehyde or a ketone.
3. MS: base peak 43 = CH_3CO^+; 57 = M − 15 ($C_2H_5CO^+$); 29 = $C_2H_5^+$. A CH_3–CO–C_2H_5 structure explains all three.
4. The data fit **butanone**, $CH_3COCH_2CH_3$. Its isomer butanal, $CH_3CH_2CH_2CHO$, could also give peaks at 29 (CHO^+) and 43 ($C_3H_7^+$), so a careful chemist would confirm with an aldehyde test or ^1H NMR. (In practice the measured spectrum of butanal has its base peak at 44, from a rearrangement beyond this course.)

Model answer: "Hexane and hex-1-ene are both colourless liquids. Explain how IR spectroscopy could distinguish them." (2 marks)

Hex-1-ene contains a C=C bond and would show an absorption at 1620–1680 cm^{-1} **[1]**; hexane has no C=C and shows no absorption in this range (both show C–H at 2850–3090 cm^{-1}) **[1]**.

Examiner traps in IR interpretation

- Quote the **bond**, not the functional group name, with its range: 'C=O at 1700–1750 cm^{-1}', not 'carbonyl peak at 1700'.
- Distinguish the two O–H rows: alcohol 3200–3600, carboxylic acid 2500–3000. Name the one that fits.
- Almost every organic compound has C–H absorptions near 3000 cm^{-1}: they cannot be used to identify a class.
- IR identifies bonds, and so functional groups; it does not usually distinguish isomers within the same class (propan-1-ol and propan-2-ol give very similar functional group regions). Use MS or NMR.
- Read the axis carefully: it runs from 4000 on the left, and the scale may change at 2000 cm^{-1}.

Practice D **Calculations and IR activity**

Answer each part.

1. Calculate the wavenumber of IR radiation of wavelength 3.45 µm.
2. Calculate the wavelength, in m, and the frequency, in s^{-1}, of radiation absorbed at 2100 cm^{-1}.
3. Which absorbs radiation of the shorter wavelength in each pair, and why? (i) C–O or C=O (ii) C–Cl or C–Br (iii) C–H or C–C
4. Which of these molecules are IR active? N_2, HCl, CO, CH_4, O_2, H_2O, Cl_2, SO_2. Explain your choice for two of them.
5. Sulfur dioxide is bent. Describe its three vibrational modes and state which are IR active.
6. State two factors that determine the global warming potential of a gas, and suggest why CFC-13 has a much higher GWP than CO_2.

Practice E **Deduce the class from the absorptions**

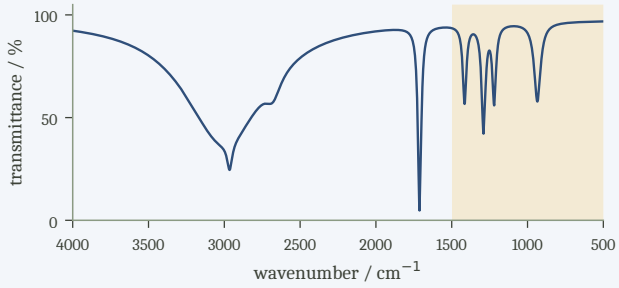
Each compound's formula and main IR absorptions (cm^{-1}) are given. Identify the bonds responsible and suggest a structure for each compound.

	Formula	Absorptions / cm^{-1}
(a)	C_3H_6O	strong, sharp 1720; 2820 and 2720 (weak); nothing at 3200–3600
(b)	C_3H_8O	broad 3200–3600; 1050–1150; no absorption at 1700–1750
(c)	$C_4H_8O_2$	very broad 2500–3300; strong 1710
(d)	C_4H_8	3080; weak 1650; 2850–2960
(e)	C_3H_9N	two medium bands at 3290 and 3370; 2850–2960
(f)	$C_4H_6O_2$	strong 1725; weak 1640; very broad 2500–3300
(g)	$C_3H_6O_2$	broad 3200–3600; strong 1715; no very broad absorption at 2500–3000

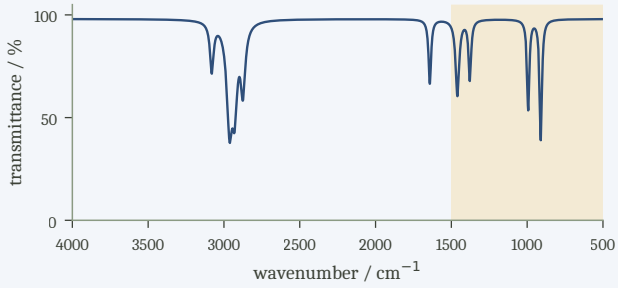
Practice F **Match the spectra to the compounds**

The IR spectra of six compounds are shown: hexane, hex-1-ene, propan-1-ol, butanal, butanoic acid and propylamine (propan-1-amine). Match each spectrum to its compound and identify the key absorption(s) that you used.

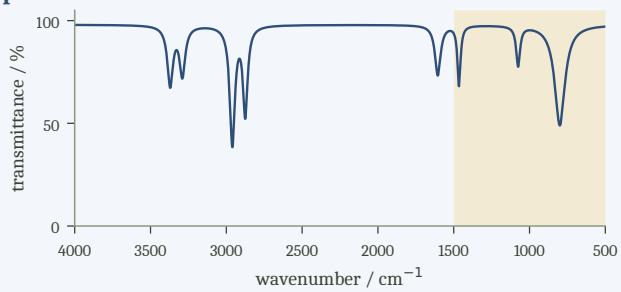
Spectrum 1



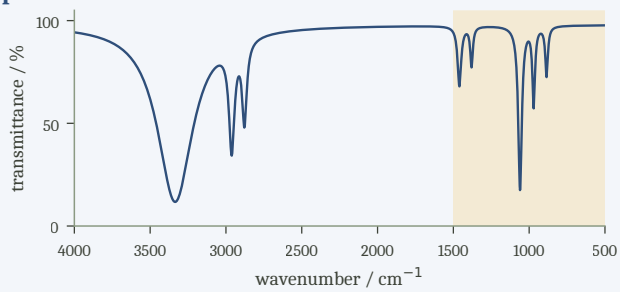
Spectrum 2



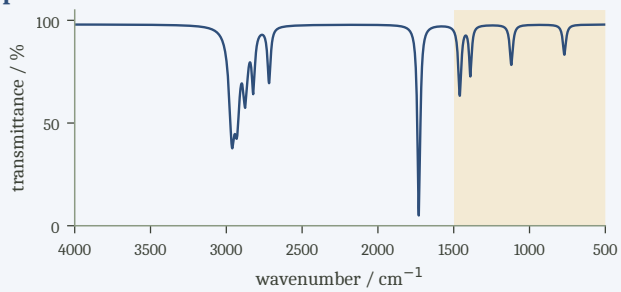
Spectrum 3



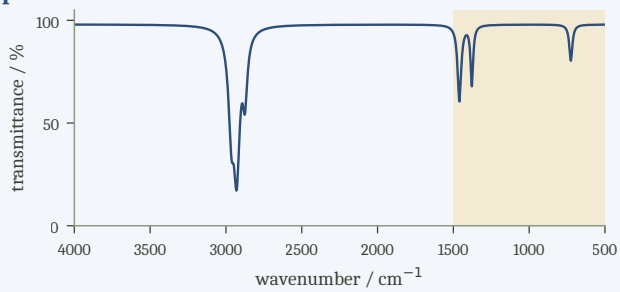
Spectrum 4



Spectrum 5



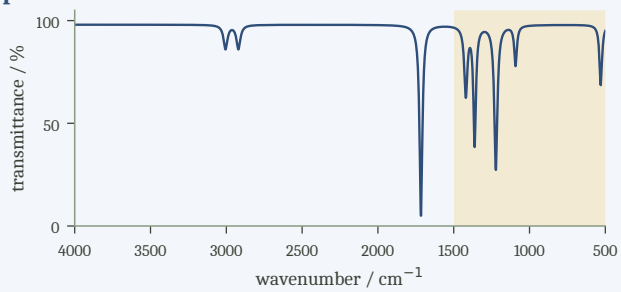
Spectrum 6



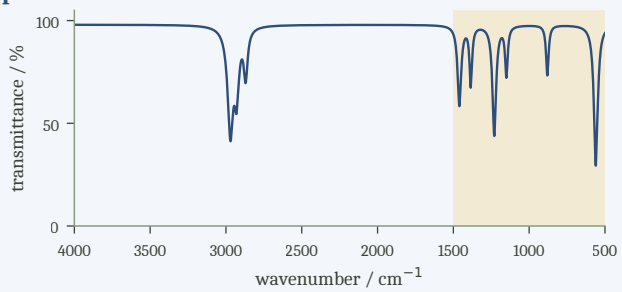
Practice G **Following a synthesis**

Propene reacts with HBr to form compound X. X reacts with aqueous sodium hydroxide to form Y, and Y is oxidized by acidified potassium dichromate(VI) to form Z, which does not react further. (a) Identify X, Y and Z. (b) The IR spectra of X, Y and Z are shown in a random order. Match them, giving your reasons.

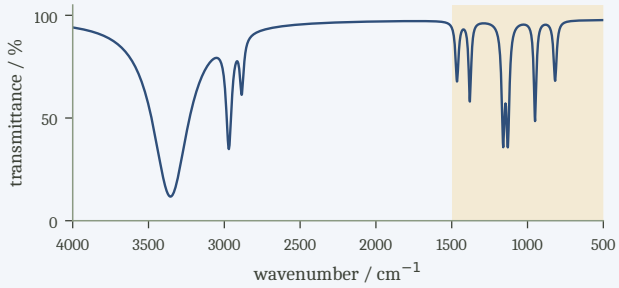
Spectrum 7



Spectrum 8



Spectrum 9



7 Key points to memorise

Everything below is either wording that examiners look for, or knowledge you must carry into the exam yourself.

A Mass spectrometry

- **Molecular ion**, M^+: molecule minus one electron; highest m/z; $m/z = M_r$. **Base peak**: tallest peak (100%), most abundant ion.
- **Fragmentation**: $M^+ \rightarrow X^+ + Y^{\bullet}$; only the ion is detected; the charge stays on the more stable fragment.
- Section 22 gives masses **lost**: 15 CH_3, 17 OH, 18 H_2O, 28 C_2H_4/CO, 29 C_2H_5/CHO, 31 OCH_3, 45 COOH.
- Common ions: 15 CH_3^+, 29 $C_2H_5^+$/CHO^+, 31 CH_2OH^+, 43 $C_3H_7^+$/CH_3CO^+, 45 $COOH^+$, 57, 77 $C_6H_5^+$.
- Isomers: same M^+, different fragmentation patterns. Always write ions with a + charge.

B IR spectroscopy

- Wavenumber (cm^{-1}) = $1/\lambda$ (cm); higher wavenumber = higher frequency and energy, shorter wavelength.
- IR radiation makes bonds vibrate (stretch, bend). Frequency rises with bond strength and falls with atomic mass.
- IR active only if the vibration **changes the dipole moment**. N_2, O_2 inactive; symmetric stretch of CO_2 inactive; all three modes of H_2O active.
- Greenhouse gases absorb long-wavelength IR from the Earth's surface. GWP depends on IR absorption and atmospheric lifetime (relative to CO_2 = 1).
- Key ranges (Section 20): O–H alcohol 3200–3600 broad; O–H acid 2500–3000 very broad; C=O 1700–1750 sharp, strong; C=C 1620–1680; C–H 2850–3090; N–H 3300–3500; C–O 1050–1410.
- Fingerprint region (below 1500): unique to each compound; used for matching and purity checks.

C Command terms — what each one is actually asking for

- **Identify** (the species responsible for a peak) — the formula of the ion, with its + charge.
- **Deduce** (the structure / molecular formula) — show the reasoning: M^+, masses lost, ions, bonds.
- **Explain** (why a molecule is IR active) — link the vibration to a change in dipole moment.
- **Outline / Explain** (how IR distinguishes two compounds) — name a bond present in one but not the other and give its wavenumber range.
- **State** (the bond responsible for an absorption) — bond and range only.

8 Check yourself

Exam-style questions on the whole booklet. Cover the answers. All questions are Higher Level.

1. What is the molecular ion of ethanol?

   A $C_2H_5OH^-$ B $C_2H_5OH^+$
   C $C_2H_5^+$ D CH_2OH^+

2. A compound has a molecular ion at m/z = 74 and a strong peak at 29. Which mass was lost to give the peak at 45?

   A 15 B 17 C 29 D 45

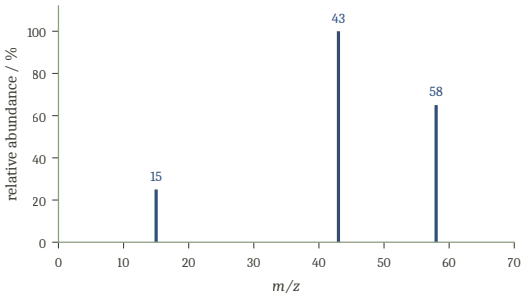
3. Which ion could be responsible for a peak at $m/z = 43$?

A $C_2H_5^+$ B CH_3CO^+
C $COOH^+$ D CH_2OH^+

4. Which compound would give a large peak at $m/z = 31$?

A propan-1-ol B propan-2-ol
C propanone D propane

5. The mass spectrum of a compound with the formula C_3H_6O is shown. Identify the species responsible for the peaks at 58, 43 and 15, and hence identify the compound. **[4]**



6. A compound with the empirical formula C_2H_4O gives a molecular ion at 88 and peaks at 71 and 45. Deduce the molecular formula and suggest a structure. **[4]**

7. Explain why the mass spectra of butane and 2-methylpropane are different, even though both have a molecular ion at $m/z = 58$. **[2]**

8. A bromoalkane gives two molecular ion peaks of equal height at $m/z = 136$ and 138. Deduce its molecular formula and draw two possible structures. **[3]**

9. Which bond absorbs IR radiation at the highest wavenumber?

A C–O B C=O C C–H D C–Br

10. Which type of bond would absorb IR radiation of the longest wavelength?

A a single bond between light atoms B a single bond between heavy atoms
C a double bond between light atoms D a double bond between heavy atoms

11. Which molecule does **not** absorb IR radiation?

A CO B CH_4 C N_2 D N_2O

12. Explain why water vapour and carbon dioxide are greenhouse gases but oxygen is not. **[3]**

13. State two factors that affect the global warming potential of a greenhouse gas. **[2]**

14. An absorption occurs at a wavelength of 5.75×10^{-6} m. Calculate its wavenumber in cm^{-1} and identify a bond that could be responsible. **[2]**

15. Explain why the O–H absorption in the IR spectrum of an alcohol is broad. **[1]**

16. The IR spectrum of a compound shows strong absorptions at 2950 and 1740 cm^{-1} and at 1240 cm^{-1}, and no absorption between 2500 and 3600 cm^{-1} apart from C–H. Which class could it belong to?

A alcohol B carboxylic acid
C ester D alkene

17. Describe how the IR spectra of propan-1-ol and propanal would differ. **[2]**

18. Explain why IR spectroscopy would not easily distinguish propan-1-ol from propan-2-ol, and suggest a technique that would. **[2]**

19. The intoximeter measures the absorbance of breath at 2950 cm^{-1}. Identify the bond responsible, and explain why water in the breath does not interfere. **[2]**

20. Compound W, $C_4H_8O_2$, shows a very broad IR absorption at 2500–3300 cm^{-1} and a strong one at 1710 cm^{-1}. Its mass spectrum shows peaks at 88, 71, 45 and 43. Deduce two possible structures of W and use the mass spectrum to suggest which group is present. **[4]**

21. A compound X contains carbon, hydrogen and oxygen only. Its IR spectrum shows a broad absorption at 3200–3600 cm^{-1} and a strong one at 1720 cm^{-1}. Its molecular ion is at $m/z = 74$, and there are peaks at 43 and 31. Suggest a structure for X and explain each piece of evidence. **[4]**

22. Outline how the fingerprint region of an IR spectrum could be used to show that a sample of aspirin is pure. **[2]**

9 Answers

Practice A — fragment ions

(a) 15 CH_3^+; 29 $C_2H_5^+$ (middle C–C breaks); 43 $C_3H_7^+$ (loss of CH_3)

(b) 15 CH_3^+; 43 CH_3CO^+ (loss of CH_3)

(c) 29 $C_2H_5^+$ or CHO^+ (C–C next to C=O breaks); 57 $C_2H_5CO^+$ (loss of H)

(d) 15 CH_3^+; 43 CH_3CO^+ (loss of OH, 17); 45 $COOH^+$ (loss of CH_3)

(e) 29 $C_2H_5^+$ (loss of OH); 31 CH_2OH^+ (loss of CH_3); 45 $C_2H_5O^+$ (loss of H)

(f) 45 CH_3CHOH^+ (loss of CH_3); 59 $(CH_3)_2COH^+$ (loss of H)

(g) 77 $C_6H_5^+$ (loss of CH_3); 91 $C_6H_5CH_2^+$ (loss of H)

(h) 29 $C_2H_5^+$; 57 $C_2H_5CO^+$ (loss of OCH_3, 31); 59 $COOCH_3^+$ (loss of C_2H_5, 29)

Practice B — identifying isomers

- **(a)** Spectrum 1 is **propan-2-ol**: base peak 45 = CH_3CHOH^+ (M − 15, loss of CH_3). Spectrum 2 is **propan-1-ol**: base peak 31 = CH_2OH^+ (M − 29, loss of C_2H_5); propan-2-ol has no CH_2OH group.
- **(b)** Spectrum 3 is **propanal**: peaks at 29 ($C_2H_5^+$ and CHO^+) and 57 (M − 1). Spectrum 4 is **propanone**: 43 = CH_3CO^+ and 15 = CH_3^+; no 29, because there is no C_2H_5 group.
- **(c)** Spectrum 5 is **propanoic acid**: 57 (M − 17, loss of OH), 45 ($COOH^+$) and 29 ($C_2H_5^+$). Spectrum 6 is **methyl ethanoate**: 43 = CH_3CO^+ (M − 31, loss of OCH_3), 59 (M − 15) and 15.

Practice C — molecular formulas and halogens

1. 84 ÷ 14 = 6: C_6H_{12}; an alkene (e.g. hex-1-ene) or a cycloalkane (cyclohexane).
2. C_3H_6O = 58; 116 ÷ 58 = 2: $C_6H_{12}O_2$.
3. C_3H_7Cl (1- or 2-chloropropane): the molecular ions contain ^{35}Cl (78) and ^{37}Cl (80), in the ratio of the isotope abundances, about 3 : 1.
4. Equal M and M+2 peaks mean one Br atom; 122 − 79 = 43, so the rest is C_3H_7: C_3H_7Br, 1-bromopropane or 2-bromopropane (43 = $C_3H_7^+$).
5. When the C–O bond breaks, the positive charge stays on the more stable fragment, $C_2H_5^+$ (29); the OH leaves as a neutral radical, which is not detected.
6. Its molecular ion fragments very easily by losing CH_3 (72 − 15 = 57), forming the stable ion $(CH_3)_3C^+$, $C_4H_9^+$; very few molecular ions reach the detector.

Practice D — calculations and IR activity

1. 3.45 µm = 3.45×10^{-4} cm; $1 \div 3.45 \times 10^{-4} = 2.90 \times 10^3$ cm^{-1} (2899 cm^{-1}, C–H).
2. $\lambda = 1/2100$ cm = 4.76×10^{-4} cm = 4.76×10^{-6} m; $f = 3.00 \times 10^8 \div 4.76 \times 10^{-6} = 6.30 \times 10^{13}$ s^{-1}.
3. (i) C=O: stronger bond, higher frequency. (ii) C–Cl: Cl is lighter than Br (and the bond is stronger). (iii) C–H: H is much lighter than C.
4. IR active: HCl, CO, CH_4, H_2O, SO_2 (each has a vibration that changes the dipole moment; HCl and CO are polar diatomics). Inactive: N_2, O_2, Cl_2 (non-polar diatomics; stretching leaves the dipole at zero).
5. Symmetric stretch, asymmetric stretch and bend, like water. SO_2 is bent, so all three change the dipole moment: all are IR active.
6. How strongly the molecule absorbs IR radiation, and its atmospheric lifetime. CFC-13 has several very polar C–F and C–Cl bonds that absorb strongly at wavelengths where CO_2 and water do not, and it persists for hundreds of years.

Practice E — deducing the class

(a) C=O, aldehyde C–H, no O–H: propanal CH_3CH_2CHO

(b) O–H (alcohol), C–O: propan-1-ol or propan-2-ol

(c) O–H (acid) + C=O: butanoic acid or 2-methylpropanoic acid

(d) =C–H (above 3000) and C=C: an alkene, e.g. but-1-ene

(e) N–H, two bands: a primary amine, e.g. propylamine $CH_3CH_2CH_2NH_2$
(f) O–H (acid), C=O and C=C: an unsaturated acid, e.g. CH_2=$CHCH_2COOH$ or CH_3CH=$CHCOOH$
(g) O–H (alcohol) and C=O, no acid O–H: a hydroxyketone or hydroxyaldehyde, e.g. 1-hydroxypropanone CH_3COCH_2OH

Practice F — matching spectra

- Spectrum 1: **butanoic acid** (very broad O–H 2500–3300, C=O 1710).
- Spectrum 2: **hex-1-ene** (=C–H just above 3000, weak C=C about 1640).
- Spectrum 3: **propylamine** (two N–H bands at 3300–3400).
- Spectrum 4: **propan-1-ol** (broad O–H 3200–3600, strong C–O near 1060, no C=O).
- Spectrum 5: **butanal** (strong C=O 1730, no O–H; the two weak bands near 2720 and 2820 are the aldehyde C–H).
- Spectrum 6: **hexane** (C–H only, 2850–2960; nothing else above 1500).

Practice G — following a synthesis

- (a) X = 2-bromopropane, $CH_3CHBrCH_3$ (Markovnikov addition); Y = propan-2-ol, $CH_3CH(OH)CH_3$; Z = propanone, CH_3COCH_3 (a secondary alcohol oxidizes to a ketone, which is not oxidized further).
- (b) Spectrum 8 is **X**: only C–H above 1500 (no O–H, no C=O); C–Br absorbs near 560 in the fingerprint region. Spectrum 9 is **Y**: broad O–H at 3200–3600 and C–O near 1150. Spectrum 7 is **Z**: strong C=O at about 1715 and no O–H.

Check yourself

1. **B.** The molecule minus one electron, with a 1+ charge.
2. **C.** 74 − 45 = 29 (loss of C_2H_5 or CHO); e.g. propanoic acid gives $COOH^+$ at 45.
3. **B.** CH_3CO^+ = 15 + 28 = 43.
4. **A.** CH_2OH^+ from a primary alcohol.
5. 58: $CH_3COCH_3^+$, molecular ion **[1]**; 43: CH_3CO^+ (loss of CH_3) **[1]**; 15: CH_3^+ **[1]**. Compound: propanone (no peak at 29, so not propanal) **[1]**.
6. 88 ÷ 44 = 2: $C_4H_8O_2$ **[1]**. 71 = M − 17 (loss of OH) **[1]**; 45 = $COOH^+$ **[1]**. A carboxylic acid: butanoic acid $CH_3CH_2CH_2COOH$ (or 2-methylpropanoic acid) **[1]**.
7. The atoms are joined differently, so different bonds break and different fragments form **[1]**; e.g. butane gives $C_2H_5^+$ at 29, which 2-methylpropane (no CH_2CH_3 group) hardly gives **[1]**.
8. Equal peaks two apart: one Br atom **[1]**; 136 − 79 = 57 = C_4H_9, so C_4H_9Br **[1]**; any two of 1-bromobutane, 2-bromobutane, 1-bromo-2-methylpropane, 2-bromo-2-methylpropane **[1]**.
9. **C.** Bonds to the light H atom absorb highest (2850–3090 cm^{-1}).
10. **B.** Weak bond and heavy atoms → lowest frequency → longest wavelength.
11. **C.** N_2 is a non-polar diatomic; no vibration changes its dipole moment.
12. Absorbing IR requires a vibration that changes the dipole moment **[1]**. H_2O (bent, polar) and CO_2 (asymmetric stretch and bends) have such vibrations, so they absorb the IR radiated by the Earth **[1]**. O_2 is non-polar and its only vibration (stretching) does not change its dipole moment **[1]**.
13. Ability to absorb IR radiation (strength / wavelengths of absorption) **[1]**; atmospheric lifetime **[1]**.
14. 5.75×10^{-4} cm; $1 \div 5.75 \times 10^{-4} = 1739\ cm^{-1}$ **[1]**; C=O (1700–1750) **[1]**.
15. Hydrogen bonding between the molecules changes the O–H vibration, giving a spread of frequencies **[1]**.
16. **C.** C=O (1740) and C–O (1240) but no O–H.

17. Propan-1-ol: broad O–H absorption at 3200–3600 cm^{-1} and no C=O **[1]**; propanal: strong C=O at 1700–1750 cm^{-1} and no O–H absorption **[1]**.

18. Both have the same bonds (O–H, C–O, C–H), so their functional group regions are almost identical **[1]**; mass spectrometry (base peak 31 against 45) or ^{1}H NMR would distinguish them **[1]**.

19. C–H (2850–3090 cm^{-1}) **[1]**; water contains no C–H bonds, so it does not absorb at this wavenumber **[1]**.

20. Carboxylic acid: O–H (acid) and C=O **[1]**; $C_4H_8O_2$ acids: butanoic acid $CH_3CH_2CH_2COOH$ and 2-methylpropanoic acid $(CH_3)_2CHCOOH$ **[1]**; 71 = M – 17 (OH lost), 45 = $COOH^+$ **[1]**; 43 = $C_3H_7^+$ (M – COOH), so a propyl or isopropyl group; MS alone does not decide **[1]**.

21. 1-Hydroxypropanone, CH_3COCH_2OH (M_r = 74) **[1]**: broad absorption at 3200–3600 = O–H (alcohol) **[1]**; 1720 = C=O **[1]**; 43 = CH_3CO^+ and 31 = CH_2OH^+, from breaking the bonds either side of the C=O **[1]**.

22. Record the spectrum of the sample and compare it with that of pure aspirin from a database **[1]**; if pure, the fingerprint regions match exactly; extra troughs indicate an impurity **[1]**.

Where this fits in Structure 3.2

- **Booklet 4** — 3.2.1 to 3.2.4: formulas, functional groups, homologous series and physical trends.
- **Booklet 5** — 3.2.5 and 3.2.6: IUPAC nomenclature and structural isomers.
- **Booklet 6** (HL) — 3.2.7: stereoisomers.
- **Booklet 7** (this booklet, HL) — 3.2.8 and 3.2.9: mass spectrometry and infrared spectroscopy.
- **Next** — HL 3.2.10 to 3.2.12: ^{1}H NMR spectroscopy, splitting patterns and combining techniques.
- Links: **Structure 1.2** (the mass spectrometer), **Structure 1.3** (electromagnetic spectrum), **Reactivity 1.3** (greenhouse gases), **Reactivity 3.2** (oxidation of alcohols, followed by IR).

These notes are a free resource, shared for any IB student who finds them useful.

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