

# Infrared Spectroscopy and Mass Spectrometry

How can chemists identify a compound's functional groups and molar mass from its spectra?

●●○ Intermediate

Analytical Chemistry

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**Before you start:** it helps to understand [Functional Groups](#) and [Light and Atomic Spectra](#).

## What is it?

**Spectroscopy** and **spectrometry** let chemists identify a compound without a chemical test, using only a few milligrams.

- **Infrared (IR) spectroscopy** shines infrared light through a sample. Covalent bonds **vibrate** (stretch and bend), and each type of bond absorbs IR at a characteristic **wavenumber**, measured in  $\text{cm}^{-1}$ . The absorptions show which **functional groups** are present.
- **Mass spectrometry (MS)** turns molecules into positive ions, breaks some of them into fragments, and sorts the ions by their **mass-to-charge ratio**,  $m/z$ . The heaviest ion usually gives the **molar mass**.

The wavenumber is the number of waves per centimetre, the reciprocal of the wavelength:  $\tilde{\nu} = 1/\lambda$ . A higher wavenumber means a higher frequency and more energy.

### 💡 KEY IDEA

IR answers “**which functional groups?**”; mass spectrometry answers “**how heavy, and in what pieces?**” Together with NMR, they let chemists work out the structure of almost any organic compound.

## Why does it matter?

- **Identifying unknowns.** Forensic laboratories, drug testing and quality control identify substances from their spectra.
- **Breathalyzers** measure ethanol in breath using its IR absorption.
- **Climate.** Carbon dioxide, methane and water vapour absorb infrared radiation from the Earth, which is the greenhouse effect.
- **Space and medicine.** Mass spectrometers analyse the atmospheres of planets, detect drugs in sport and identify proteins in disease.

# How does it work?

## 1. Reading an IR spectrum

An IR spectrum plots **transmittance** (%) against **wavenumber**, with wavenumber decreasing from left (about  $4000\text{ cm}^{-1}$ ) to right (about  $500\text{ cm}^{-1}$ ). Absorptions appear as **dips** (“peaks” pointing down).

| Bond                     | Where found                       | Wavenumber ( $\text{cm}^{-1}$ ) | Appearance           |
|--------------------------|-----------------------------------|---------------------------------|----------------------|
| O-H                      | alcohols                          | 3200–3550                       | strong, <b>broad</b> |
| O-H                      | carboxylic acids                  | 2500–3300                       | very broad           |
| N-H                      | amines, amides                    | 3300–3500                       | medium               |
| C-H                      | almost all organic compounds      | 2850–3100                       | medium–strong        |
| $\text{C}\equiv\text{N}$ | nitriles                          | about 2250                      | medium, sharp        |
| C=O                      | aldehydes, ketones, acids, esters | 1680–1750                       | <b>strong, sharp</b> |
| C=C                      | alkenes                           | 1620–1680                       | weak–medium          |
| C-O                      | alcohols, esters, ethers          | 1000–1300                       | strong               |

The region below about  $1500\text{ cm}^{-1}$  contains many overlapping absorptions. It is called the **fingerprint region**: it is unique to each compound, so it can be matched against a database to confirm an identity.

## 2. Reading a mass spectrum

A mass spectrum is a bar chart of **relative abundance** against  $m/z$  (for ions with a 1+ charge,  $m/z$  is simply the mass).

- The **molecular ion**,  $\text{M}^+$ , is the peak at the highest  $m/z$  (ignoring small isotope peaks). Its  $m/z$  equals the **molar mass**.
- The tallest peak is the **base peak** (set to 100 %). It comes from the most stable fragment.
- **Fragments** reveal pieces of the molecule:  $m/z$  15 ( $\text{CH}_3^+$ ), 29 ( $\text{C}_2\text{H}_5^+$  or  $\text{CHO}^+$ ), 31 ( $\text{CH}_2\text{OH}^+$ ), 43 ( $\text{C}_3\text{H}_7^+$  or  $\text{CH}_3\text{CO}^+$ ), 45 ( $\text{COOH}^+$ ).
- **Isotope patterns**: a compound with one Cl atom shows peaks at M and M+2 in a **3 : 1** ratio ( $^{35}\text{Cl}$  and  $^{37}\text{Cl}$ ); one Br atom gives M and M+2 in a **1 : 1** ratio.

### ∞ THINK OF IT LIKE THIS

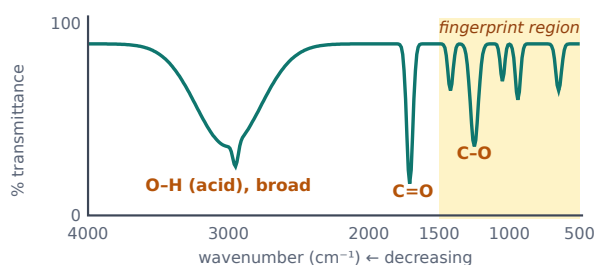
IR spectroscopy is like listening to an orchestra: each type of bond “plays” at its own pitch, so you can hear which instruments (functional groups) are present. Mass spectrometry is like weighing a vase and then the pieces it breaks into: the whole vase gives the total mass, and the pieces hint at how it was put together.

### Q MORE PRECISELY

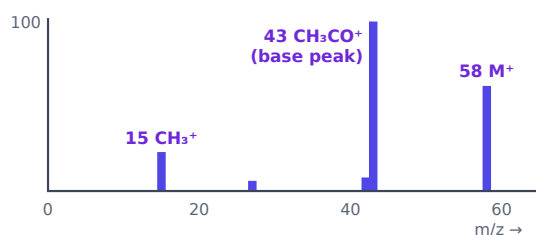
A bond absorbs IR only if its vibration **changes the dipole moment** of the molecule, which is why  $\text{N}_2$  and  $\text{O}_2$  do not absorb but  $\text{CO}_2$  and  $\text{H}_2\text{O}$  do. Stronger bonds and lighter atoms vibrate faster, so they absorb at higher wavenumbers:  $\text{C}\equiv\text{C}$  absorbs higher than  $\text{C}=\text{C}$ , which absorbs higher than  $\text{C}-\text{C}$ . In MS, the most common method (electron impact) knocks an electron out of the molecule; the small  $M+1$  peak comes mainly from carbon-13 (1.1 % of carbon atoms), and high-resolution MS measures masses to four decimal places, enough to fix the molecular formula.

## Visualise it

IR spectrum: ethanoic acid (schematic)



Mass spectrum: propanone,  $\text{CH}_3\text{COCH}_3$  (scheme)



Top: IR spectrum of ethanoic acid. Bottom: mass spectrum of propanone. (Schematic.)

## Worked example

### ✏ WORKED EXAMPLE: Wavenumber and wavelength

**Question:** A  $\text{C}=\text{O}$  absorption appears at  $1715\text{ cm}^{-1}$ . What is its wavelength in micrometres?

$$\begin{aligned}\lambda &= \frac{1}{\tilde{\nu}} = \frac{1}{1715\text{ cm}^{-1}} \\ &= 5.831 \times 10^{-4}\text{ cm} \\ &= 5.831 \times 10^{-4}\text{ cm} \\ &\quad \times \frac{10^4\text{ }\mu\text{m}}{1\text{ cm}} = 5.83\text{ }\mu\text{m}\end{aligned}$$

 **WORKED EXAMPLE:** Alcohol, acid or ketone?

**Question:** Three compounds give these IR absorptions. Identify the functional group in each. (a) broad  $3350\text{ cm}^{-1}$ ,  $1050\text{ cm}^{-1}$ , nothing near  $1700\text{ cm}^{-1}$  (b) very broad  $2500\text{--}3300\text{ cm}^{-1}$  and strong  $1710\text{ cm}^{-1}$  (c) strong  $1715\text{ cm}^{-1}$ , no absorption above  $3100\text{ cm}^{-1}$

**Step 1** (a) O–H (alcohol) and C–O, no C=O: an **alcohol**.

**Step 2** (b) Very broad acid O–H plus C=O: a **carboxylic acid**.

**Step 3** (c) C=O but no O–H: a **ketone** or **aldehyde** (or ester).

 **WORKED EXAMPLE:** Average atomic mass from a mass spectrum

**Question:** The mass spectrum of chlorine atoms shows  $^{35}\text{Cl}$  (34.969, 75.76 %) and  $^{37}\text{Cl}$  (36.966, 24.24 %). Calculate the relative atomic mass of chlorine.

$$\begin{aligned}A_r &= 34.969 \\&\quad \times 0.7576 + 36.966 \times 0.2424 \\&= 35.45\end{aligned}$$

The 3 : 1 ratio of the isotopes is why chlorine compounds show M and M+2 peaks in a 3 : 1 ratio.

 **WORKED EXAMPLE:** Putting IR and MS together

**Question:** An unknown has the formula  $\text{C}_3\text{H}_6\text{O}$ . Its IR spectrum shows a strong absorption at  $1715\text{ cm}^{-1}$  and none at  $3200\text{--}3550\text{ cm}^{-1}$ . Its mass spectrum shows  $M^+$  at  $m/z$  58 and the base peak at  $m/z$  43. Identify it.

**Step 1**  $M^+ = 58$  matches  $\text{C}_3\text{H}_6\text{O}$  (58.08 g/mol).

**Step 2** IR: C=O present, no O–H: an aldehyde or a ketone.

**Step 3** MS: a base peak at 43 is  $\text{CH}_3\text{CO}^+$ , formed when the molecule loses  $\text{CH}_3$  ( $58 - 15 = 43$ ).

**Step 4** The compound is **propanone**,  $\text{CH}_3\text{COCH}_3$ . (Its isomer propanal would give a strong peak at 29,  $\text{CHO}^+$  or  $\text{C}_2\text{H}_5^+$ .)

## Common mistake

 **COMMON MISTAKE:** Reading the wavenumber axis the wrong way

IR spectra are drawn with wavenumber **decreasing** from left to right. An O–H band near  $3300\text{ cm}^{-1}$  is on the **left**; C=O near  $1700\text{ cm}^{-1}$  is in the middle.

 **COMMON MISTAKE:** Taking the tallest peak as the molar mass

The tallest peak is the **base peak**, usually a fragment. The molar mass is given by the **molecular ion**, the peak at the highest  $m/z$  (apart from small isotope peaks).

 **COMMON MISTAKE:** Trying to identify everything in the fingerprint region

Below  $1500\text{ cm}^{-1}$  the absorptions overlap. Use the fingerprint region to **match** a known spectrum, and the region above  $1500\text{ cm}^{-1}$  to identify functional groups.

 **NOTATION NOTE**

- Wavenumber:  $\tilde{\nu}$ , in  $\text{cm}^{-1}$  (read “per centimetre” or “reciprocal centimetres”).
- $M^+$ : molecular ion;  $M+2$ : an ion 2 mass units heavier, usually from an isotope.

## Remember this

 **REMEMBER THIS**

- IR: bonds absorb at characteristic wavenumbers. Broad  $3200\text{--}3550$ : alcohol O–H. Very broad  $2500\text{--}3300$ : acid O–H. Strong  $1680\text{--}1750$ : C=O.
- Below  $1500\text{ cm}^{-1}$ : fingerprint region, unique to each compound.
- MS: molecular ion (highest  $m/z$ ) = molar mass; base peak = tallest; fragments show pieces.
- Cl:  $M$  and  $M+2$  in 3 : 1; Br: 1 : 1.
- Combine: MS gives the mass, IR the functional groups, NMR the carbon–hydrogen framework.

## References

1. Brown, T. L.; LeMay, H. E., Jr.; Bursten, B. E.; Murphy, C. J.; Woodward, P. M.; Stoltzfus, M. W. Chemistry: The Central Science, 15th ed.; Pearson, 2022.

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