SPECTROSCOPY

IR Spectroscopy

Infrared (IR) spectroscopy involves the interaction of infrared radiation with organic molecules. It is commonly used to identify functional groups present in organic compounds. The typical wavenumber range used in IR spectroscopy lies between 4000 cm^{-1} and 625 cm^{-1}.

IR spectroscopy is widely applied in both organic and inorganic chemistry for molecular structure analysis, demonstrating high scan speed, resolution, and sensitivity.

Principle of IR Spectroscopy

When an organic molecule containing functional groups with heteroatoms is exposed to IR radiation, the electric field component of the radiation interacts with the **dipole moment** of the molecule.

- Absorption occurs when the **frequency of IR radiation matches the natural vibrational frequency** of a bond within the molecule.
- The absorbed energy causes the bonds to **vibrate with greater amplitude**, resulting in a change in dipole moment.
- **More polar bonds absorb more intensely**.

The frequencies absorbed are characteristic of specific functional groups and molecular structures. Analysis of these frequencies allows determination of the compound's functional groups.

Components of an IR Spectrophotometer

- Source of IR radiations
- Monochromator
- Sample chamber
- Detector
- Data collection and processing system

Reading an IR Spectrum

To interpret an IR spectrum, absorption bands must be examined to identify the functional groups present in the compound.

- Each peak in an IR spectrum corresponds to a specific bond vibration, providing a molecular fingerprint.
- Compare major peaks with reference absorption values of known functional groups such as C–H, C=O, O–H, and N–H.
- The region below 1500 cm^{-1}, known as the fingerprint region, is unique for each compound and aids in identification.

Common Functional Groups and Their IR Absorption Ranges

Table 18.1: Functional Groups, Wavenumbers & Intensities

Functional Group	Bond	Wavenumber (cm^{-1})	Intensity
Alkyl	C–H	2853–2962	Medium–Strong
Alkenyl	=C–H	3010–3095	Medium
	C=C	1620–1680	Variable
Alkynyl	≡C–H	3300	Strong
	C≡C	2100–2260	Variable
Aromatic	Ar–H	3030	Variable
	C=C	1400–1600	Variable
Alcohols, Phenols, Carboxylic Acids	O–H (alcohols/phenols)	3200–3500	Broad, Strong
	O–H (carboxylic acids)	2500–3000	Broad, Variable
	C–H (alcohols)	1025–1060	Strong
Carbonyl Compounds	C=O (aldehydes)	1690–1740	Strong
	C=O (ketones)	1680–1750	Strong
	C=O (esters)	1735–1750	Strong
	C=O (carboxylic acids)	1710–1780	Strong
	C=O (amides)	1630–1690	Strong
Amines	N–H	3300–3500	Medium

IR Spectrum Examples

Interpret the IR spectrum of ethanol (C_2H_5OH).

Problem-Solving Strategy

Ch#18: Spectroscopy **By: Sir Amjad (Lecturer Chemistry)**

1. Identify the **significant absorption peaks** in the IR spectrum.
2. Compare these peaks with **standard wavenumber ranges** of functional groups.
3. Use the matched peaks to **identify and confirm functional groups** present in the molecule.

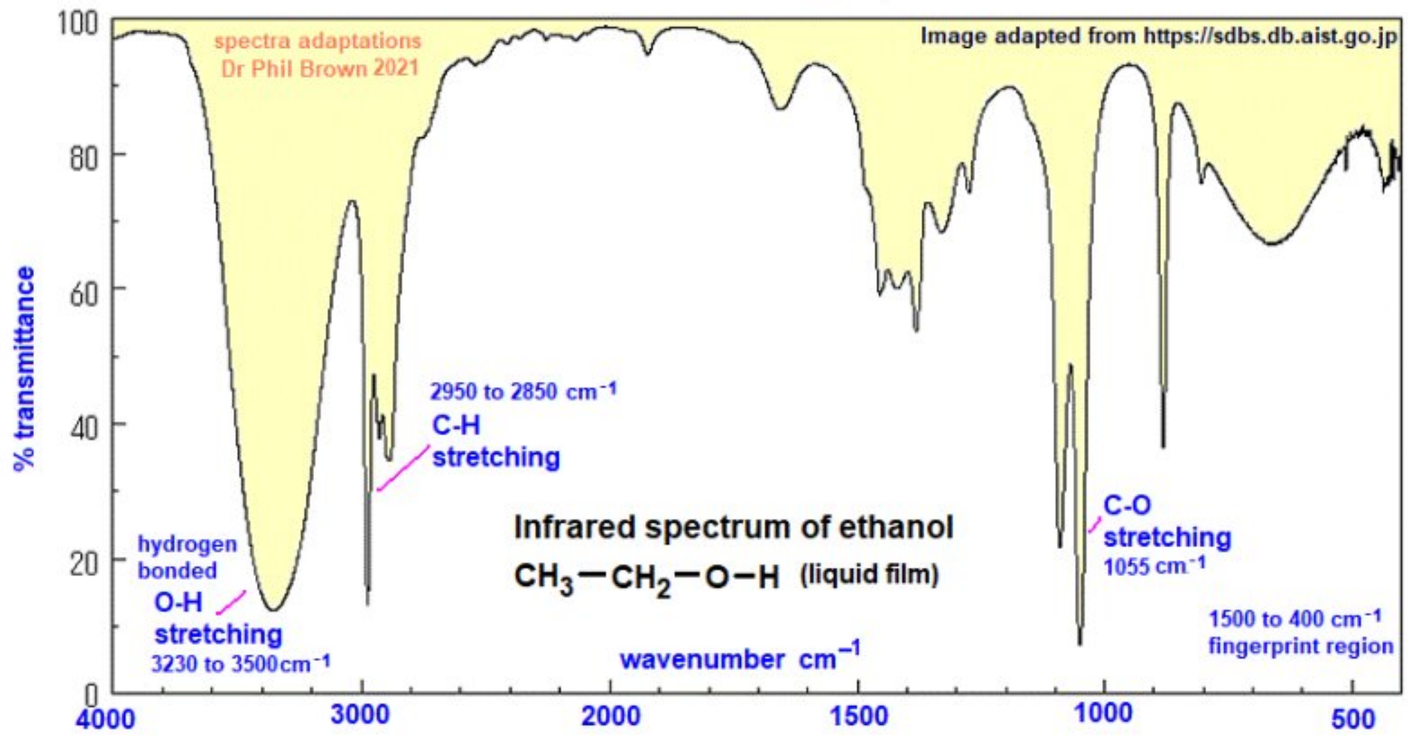
This method helps in identifying functional groups in simple molecules using IR spectroscopy.

Important Features of IR Spectrum of Ethanol (Vapour)

Wavenumber (cm^{-1})	Type of Vibration	Functional Group
~3300	Broad stretching	O–H (alcohol)
2850–2960	Stretching	C–H (alkyl group)
1050–1150	Stretching	C–O (alcohol)
1500–400	Various modes	Fingerprint region

Interpretation of Peaks

- **Broad peak around 3300 cm^{-1}**
  - Indicates **O–H stretching vibration**
  - Confirms the presence of an **alcohol functional group**
- **Peaks between 2850–2960 cm^{-1}**
  - Correspond to **C–H stretching vibrations**
  - Show the presence of an **ethyl group (C_2H_5)**
- **Peak around 1050–1150 cm^{-1}**
  - Due to **C–O stretching vibration**
  - Further supports the presence of an **alcohol**

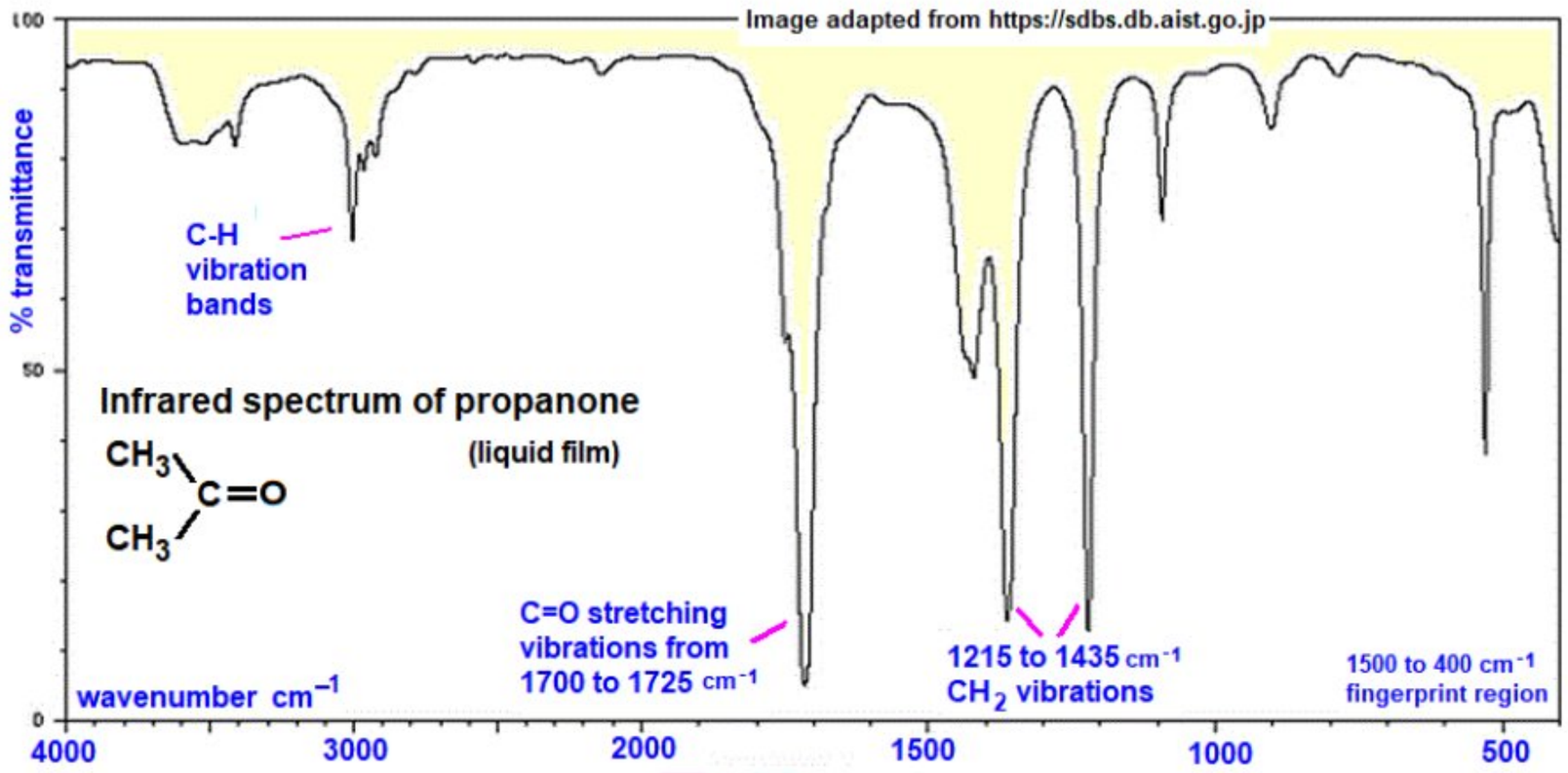


IR Spectrum of Acetone

The IR spectrum of acetone shows:

- A strong C=O absorption peak at 1700–1725 cm^{-1}
- CH_2 vibrations around 1215 cm^{-1}
- C–H stretching vibrations close to 3000 cm^{-1}

This carbonyl absorption may slightly shift in aldehydes, carboxylic acids, and related derivatives.

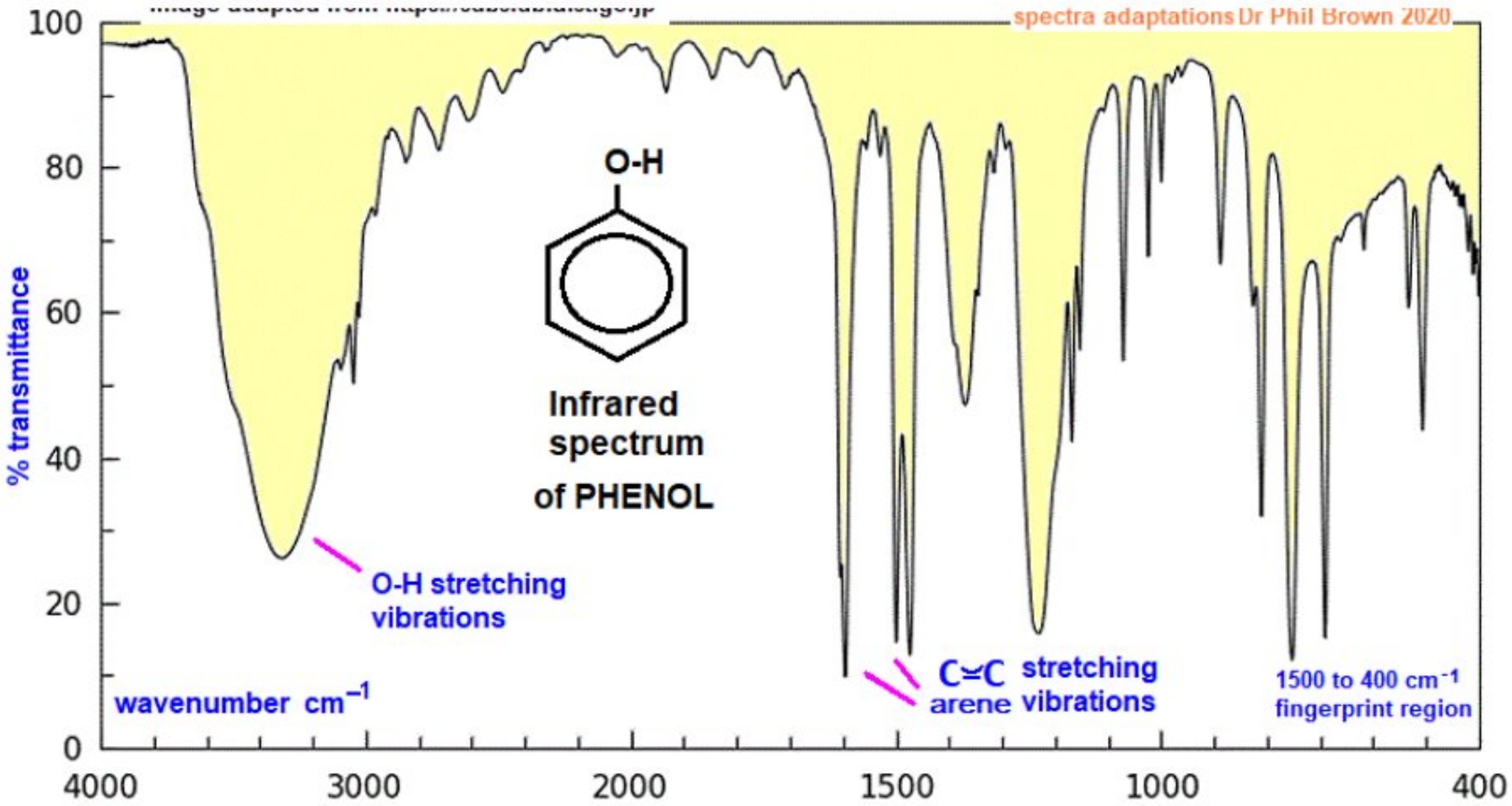


IR Spectrum of Phenol

The IR spectrum of phenol displays:

- A broad and strong O–H absorption peak, representing the presence of a hydroxyl group attached to an aromatic ring
- Absorption near 1500 cm^{-1} due to conjugated C=C aromatic bonds

Each spectral peak corresponds to a specific bond vibration, enabling identification of the compound.



UV-Visible Spectroscopy

UV-Visible spectroscopy is an analytical technique in which the absorption of ultraviolet (UV) and visible light by a compound is measured. The typical wavelength range used is 200 nm to 800 nm.

This method is based on electronic excitation: when a compound absorbs UV or visible light, electrons are promoted from lower-energy orbitals to higher-energy orbitals. The amount of absorbed light is directly proportional to the concentration of the sample containing electrons available for excitation.

UV-Visible spectroscopy is widely used in material science, chemistry, and biochemistry, and can be applied to liquid, solid and gaseous samples.

Electronic Transitions in UV-Visible Spectroscopy

Electronic excitations occur when electrons move between molecular orbitals. Common transitions include:

Transition Type	Description
$\pi \rightarrow \pi^*$	Pi to pi-star transition
$n \rightarrow \pi^*$	Non-bonding to pi-star transition
$\sigma \rightarrow \sigma^*$	Sigma to sigma-star transition
$n \rightarrow \sigma^*$	Non-bonding to sigma-star transition

These transitions occur at specific wavelengths, allowing structural information to be determined, especially about **conjugation and unsaturation** in molecules.

Colour and Light Absorption

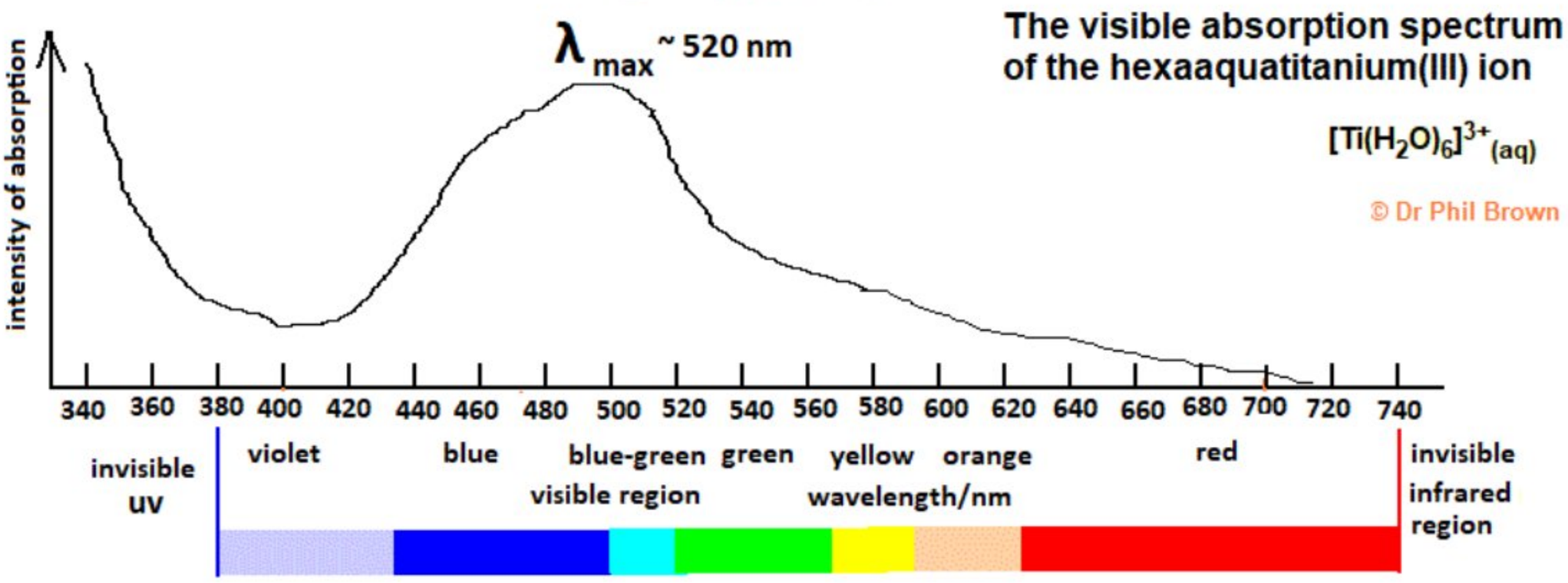
- **Coloured compounds** absorb wavelengths within the visible region (400–800 nm) and **transmit or reflect** the remaining wavelengths, which produce the observed colour.
- The colour of a compound is **not predicted by the absorbed wavelength**, but by the **transmitted or reflected wavelength**.
- Shorter wavelengths correspond to **blue/violet** region and longer wavelengths to **red/orange** region.
- A compound appears in the **complementary colour** of the wavelength it absorbs.

Table 18.2: Wavelength Absorbed vs Observed Colour

Wavelength Absorbed (nm)	Colour Observed	Colour Absorbed
400–435	Yellow-Green	Violet
435–480	Yellow	Blue
480–490	Orange	Green-Blue
490–500	Red	Blue-Green
500–560	Purple	Green
560–580	Violet	Yellow-Green
580–595	Blue	Yellow
595–605	Green-Blue	Orange
605–700	Blue-Green	Red

Example: Hexaaqua Titanium (III) Complex

The compound **$[Ti(H_2O)_6]^{3+}$** appears **violet** because it absorbs **yellow and green** wavelengths from visible light; the remaining transmitted colour is violet.



Quantitative Applications: Determining Concentration

UV-Visible spectroscopy can determine the concentration of a solution of unknown concentration using standard calibration curves:

1. **Prepare standard solutions** and measure absorbance at a specific wavelength.
2. **Plot a standard curve** (absorbance vs concentration).
3. **Measure absorbance of unknown** solution.
4. **Compare it with standard curve** to calculate concentration (Beer-Lambert Law).

Predicting UV-Visible Absorption

A compound is likely to absorb in the UV-Visible range if it contains:

- **Conjugated double bonds**
- **Aromatic rings**
- **Carbonyl groups or chromophores**
- **Electrons involved in $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$** transitions

Examples

Compound	Reason for Absorption	Approx. λmax (nm)
Benzene (C_6H_6)	Conjugated π system, $\pi \rightarrow \pi^*$ transitions	~254 nm
1,3-Butadiene (C_4H_6)	Conjugated double bonds	~217 nm
Acetone (CH_3COCH_3)	$n \rightarrow \pi^*$ transition of carbonyl group	~279 nm

Prediction of UV–Visible Absorption of a Compound

To predict whether a compound will absorb radiation in the **UV–visible region (200–800 nm)**, its **electronic structure** must be considered. Absorption occurs when electrons are promoted from a lower-energy orbital to a higher-energy orbital. The most relevant electronic transitions are:

- **$\sigma \rightarrow \sigma^*$** (very high energy; usually below 200 nm)
- **$n \rightarrow \sigma^*$** (UV region)
- **$\pi \rightarrow \pi^*$** (UV–visible region)
- **$n \rightarrow \pi^*$** (UV–visible region)

Compounds are likely to absorb in the UV–visible region if they contain:

- **Conjugated double bonds**
- **Aromatic rings**
- **Functional groups with lone-pair electrons** (e.g., carbonyl groups)

Examples

Example 1: Benzene (C_6H_6)

- Benzene has a **conjugated π-electron system** with alternating double bonds.
- It undergoes **$\pi \rightarrow \pi^*$** electronic transitions.

- **Absorption:** UV region at approximately **254 nm**.

Example 2: 1,3-Butadiene (C_4H_6)

- 1,3-Butadiene contains a **conjugated system of double bonds (C=C–C=C)**.
- Conjugation lowers the energy gap between π and π* orbitals.
- It shows **π → π*** transitions.
- **Absorption:** UV region at approximately **217 nm**.

Example 3: Acetone (CH_3COCH_3)

- Acetone contains a **carbonyl group (C=O)** with non-bonding (n) electrons on oxygen.
- It undergoes **n → π*** electronic transitions.
- **Absorption:** UV region at approximately **279 nm**.

Atomic Emission Spectroscopy (AES)

Atomic Emission Spectroscopy is an analytical technique used to **identify and quantify elements** by measuring the **specific wavelengths of light emitted** by atoms in an excited state.

Principle

When atoms of an element are supplied with sufficient energy, their electrons are excited from the ground state to higher energy levels. These excited atoms are unstable. When the excitation source is removed, electrons return to lower energy levels or the ground state and **emit energy in the form of light (photons)**.

The **wavelength of the emitted light** depends on the energy difference between the two electronic levels. Since each element has a unique electronic structure, it emits light at **characteristic wavelengths**, which can be used for identification.

Source of Excitation

Atoms may be excited using:

- Flame
- Plasma
- Electric arc
- Electric spark

Working of AES

1. The sample is converted into free atoms and excited by an energy source.
2. Excited atoms emit light during de-excitation.
3. The emitted light is passed through a **prism or diffraction grating**, which separates it into individual wavelengths.
4. A **detector** measures the intensity of emitted light.
5. The wavelength identifies the element, while the intensity indicates its concentration.

Emission Spectrum

- Appears as a **series of bright, discrete lines** on a dark background.
- Each line corresponds to a specific electronic transition.
- These lines are called **spectral lines**.
- The emission spectrum of an element acts as its **atomic fingerprint**.

Atomic Absorption Spectrum (AAS)

An **atomic absorption spectrum** is produced when **free atoms in the ground state absorb specific wavelengths of light** and get excited to higher energy levels.

Characteristics

- Absorption of light produces **dark lines** at specific wavelengths.
- These dark lines correspond exactly to the wavelengths emitted by the same element in its emission spectrum.

Comparison of Atomic Emission and Absorption Spectra

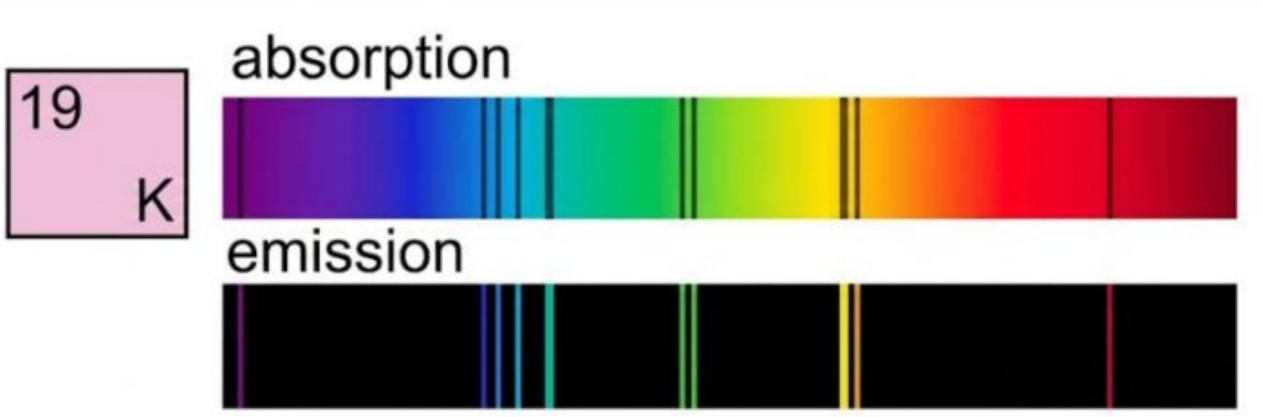
Feature	Atomic Emission Spectrum	Atomic Absorption Spectrum
Appearance	Bright lines on dark background	Dark lines on bright background
Atomic state	Excited atoms	Ground-state atoms
Process	Emission of photons	Absorption of photons
Spectral line positions	Same as absorption spectrum	Same as emission spectrum

Example: Potassium (K)

The **positions of spectral lines** (wavelengths) in both emission and absorption spectra of potassium are identical.
The only difference is:

- **Emission spectrum:** bright lines
- **Absorption spectrum:** dark lines

Thus, **atomic emission and absorption spectra are always line spectra and provide the same qualitative information about atomic energy levels**.



Nuclear Magnetic Resonance Spectroscopy (NMR)

Nuclear Magnetic Resonance (NMR) spectroscopy, also known as magnetic resonance spectroscopy (MRS), is an analytical technique used to determine the structure of molecules, particularly organic compounds. It is based on the behavior of atomic nuclei with non-zero nuclear spin when placed in an external magnetic field.

When such nuclei are exposed to a strong magnetic field and radiofrequency (RF) radiation (approximately 4–900 MHz), they absorb energy and undergo resonance. The exact resonance frequency depends on:

- The type of nucleus (isotope)
- The strength of the magnetic field
- The chemical environment of the nucleus

Because different functional groups create different chemical environments, NMR spectra are highly characteristic, making NMR one of the most powerful tools for molecular identification and structural analysis.

Principle of NMR

Certain nuclei behave as tiny nuclear magnets due to their intrinsic property called spin. In the absence of an external magnetic field, these nuclear spins are randomly oriented.

When an external magnetic field (B_0) is applied:

- The nuclei align themselves in two possible orientations:
  1. Low-energy state: spin aligned with the magnetic field
  2. High-energy state: spin aligned against the magnetic field

The energy difference (ΔE) between these two spin states corresponds to energy in the radiofrequency region.

Resonance Process

- When radiofrequency radiation of the correct energy is applied, nuclei absorb energy and flip from the low-energy state to the high-energy state.
- This absorption is called nuclear magnetic resonance.
- When the excited nuclei return to the lower energy state, they emit RF energy.
- The emitted signal is detected and recorded as an NMR spectrum.

NMR-Active Nuclei

NMR-active nuclei are those that possess:

- A non-zero nuclear spin quantum number ($I \neq 0$)
- A magnetic dipole moment

These properties allow the nucleus to interact with an external magnetic field and produce an NMR signal.

Common NMR-Active Nuclei

Nucleus	Symbol	Use
Hydrogen	^{1}H	Most common in organic chemistry
Carbon-13	^{13}C	Carbon framework analysis
Fluorine-19	^{19}F	Fluorinated compounds
Phosphorus-31	^{31}P	Phosphorus-containing compounds

Organic chemists mainly use **^{1}H NMR** and **^{13}C NMR**.

Nuclear Spin and NMR Activity

- A nucleus is NMR-active if it has a non-zero spin quantum number (I).
- Atoms with:
  - An odd number of protons, or
  - An odd number of neutrons, or
  - An odd total of protons + neutrons

have half-integer spin values such as:

- ½, 3⁄2, 5⁄2, etc.

These nuclei can absorb RF radiation and are observable in NMR.

Importance of NMR Spectroscopy

- Identifies functional groups
- Determines molecular structure
- Distinguishes between isomers
- Provides information about connectivity of atoms

Because NMR spectra are unique and highly characteristic, NMR spectroscopy is one of the most important techniques in organic chemistry.

^{1}H NMR (Proton Nuclear Magnetic Resonance)

^{1}H NMR spectroscopy is the application of nuclear magnetic resonance to **hydrogen-1 (^{1}H) nuclei** present in molecules. It is used to **determine the structure of organic compounds** by providing information about:

- Number of different types of hydrogen atoms
- Their chemical environment
- Relative number of protons
- Neighbouring atoms

Use of Deuterated Solvents

In proton NMR, deuterated solvents are used to avoid interference from solvent protons.

Why deuterated solvents are used:

- Ordinary solvents contain hydrogen, which would give extra peaks in the ^{1}H NMR spectrum.
- Deuterium (^{2}H or D) is NMR-inactive in ^{1}H NMR, so it does not interfere.

Common deuterated solvents:

- Deuterated water: **D_2O**
-
- Deuterated acetone: **$(CD_3)_2CO$**
- Deuterated chloroform: **$CDCl_3$**

Non-hydrogen solvents:

- **CS_2** and **CCl_4** may also be used because they contain no hydrogen atoms.

Tetramethylsilane (TMS) as Standard

Tetramethylsilane (TMS), $Si(CH_3)_4$, is used as the standard reference compound in proton NMR.

Reasons for using TMS:

- All 12 protons are chemically equivalent
- Produces a single sharp peak
- Protons are highly shielded due to low electronegativity of silicon
- Does not react with most organic compounds
- Volatile and easily removed

Chemical Shift Reference:

- TMS signal is assigned **$\delta = 0$ ppm**
- All other proton signals are measured **relative to TMS**

Typical Chemical Shift Range:

- Most organic protons appear between **$\delta = -4$ to $+14$ ppm**

Nuclear Spin Flipping and Chemical Shift

When a proton is placed in an external magnetic field (B_0):

- It can exist in two spin states:
  - Lower energy ($m = +½$) aligned with B_0
  - Higher energy ($m = -½$) opposed to B_0

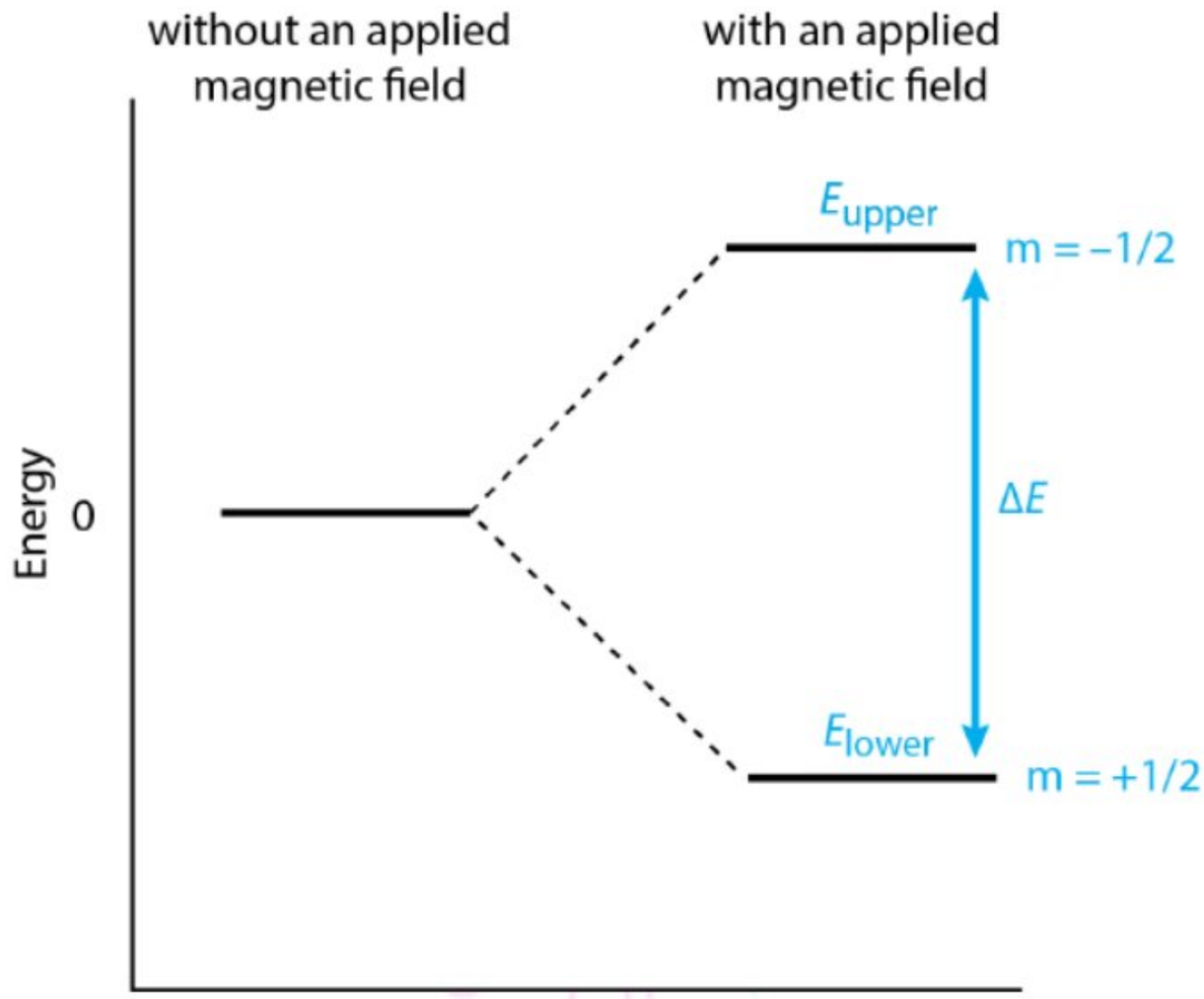
When irradiated with radiofrequency radiation of appropriate energy:

- The proton absorbs energy
- Flips from lower to higher energy state
- This transition produces an NMR signal

Chemical Shift (δ)

- The chemical shift is the difference between the resonance frequency of a proton and TMS.

- It is expressed in parts per million (ppm).
- Depends on:
  - Electronic environment
  - Shielding and deshielding effects



Shielding and Deshielding

- Shielding: High electron density around proton → less external magnetic field felt → signal appears upfield (low ppm)
- Deshielding: Low electron density (near electronegative atoms) → more external magnetic field felt → signal appears downfield (high ppm)

Example: Proton NMR of Ethyl Chloride (C_2H_5Cl)

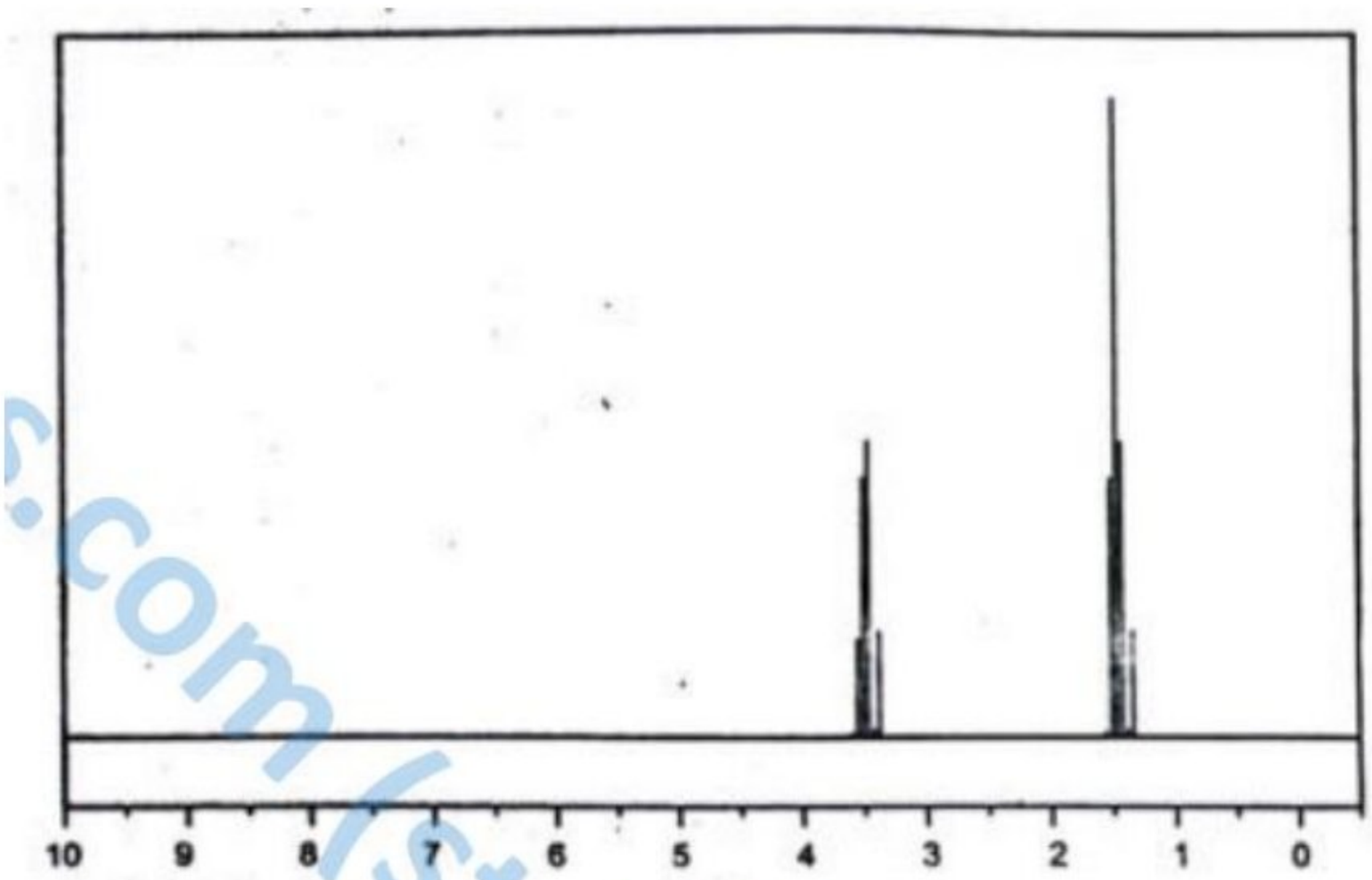
- Two different proton environments:
  - **CH_3 (methyl)** protons → signal at **~1.5 ppm**
  - **CH_2 (methylene)** protons → signal at **~3.5 ppm**

Explanation:

- CH_2 protons are closer to electronegative chlorine → more deshielded → higher ppm
- CH_3 protons are further away → more shielded → lower ppm

Splitting:

- CH_3 peak → **triplet** (due to 2 neighbouring CH_2 protons)
- CH_2 peak → **quartet** (due to 3 neighbouring CH_3 protons)



Proton NMR of Benzene

- All six protons are chemically equivalent
- Only one signal appears at ~7.2 ppm
- Due to diamagnetic ring current in aromatic system

Environment of a Proton (Multiplicity)

Protons in the same chemical environment give one signal.
Protons in different environments give separate signals.

Spin–Spin Coupling (Signal Splitting)

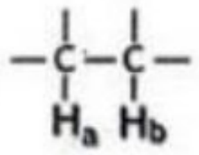
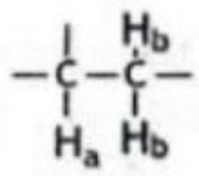
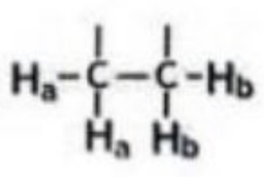
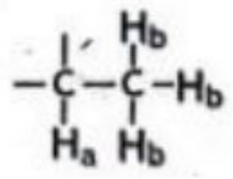
Splitting depends on the number of adjacent (neighbouring) protons.

(n + 1) Rule:

If a proton has **n neighbouring protons**, its signal splits into **(n + 1) peaks**.

Summary of Signal Splitting Patterns in ^1H NMR Spectroscopy

The pattern is that n protons split the signal into n+1 peaks, which is known as the **n+1 rule.**

Multiplicity	N + 1	H_a	Signal	H_b	N + 1	Multiplicity
Doublet	1 + 1 = 2				1 + 1 = 2	Doublet
Triplet	2 + 1 = 3				1 + 1 = 2	Doublet
Triplet	2 + 1 = 3				2 + 1 = 3	Triplet
Quartet	3 + 1 = 4				1 + 1 = 2	Doublet

Proton Exchange with D_2O

When a compound containing **O–H or N–H protons** is shaken with **D_2O**:

- The hydrogen exchanges with deuterium
- The O–H or N–H peak **disappears** from the ^1H NMR spectrum

Importance:

- Confirms the presence of:
  - Alcohols (O–H)
  - Phenols (O–H)
  - Amines (N–H)
  - Carboxylic acids (O–H)

This occurs because **deuterium is NMR inactive** in proton NMR.

Carbon-13 NMR (^{13}C-NMR)

Naturally occurring carbon consists mainly of two isotopes:

- **Carbon-12 (^{12}C)** ≈ 99% (NMR inactive)
- **Carbon-13 (^{13}C)** ≈ 1% (NMR active)
  (Trace amounts of radioactive ^{14}C are also present.)

^{13}C-NMR spectroscopy is based on the magnetic properties of the **^{13}C nucleus**.
^{13}C nuclei possess nuclear spin and therefore behave like tiny magnets, whereas ^{12}C nuclei do not show this property and are NMR inactive.

When a ^{13}C nucleus is placed in an external magnetic field (**B_0**), it can align:

- **With the magnetic field** (lower energy, more stable)
- **Against the magnetic field** (higher energy, less stable)

If radio-frequency radiation of exactly the right energy is applied, the ^{13}C nucleus flips from the lower-energy state to the higher-energy state. This phenomenon is called **resonance**, and it is detected as a **peak in the NMR spectrum**.

Chemical Shift in ^{13}C-NMR

The position of a peak in a ^{13}C-NMR spectrum is expressed as **chemical shift (δ)** and is measured in **parts per million (ppm)** relative to **TMS (tetramethylsilane)**.

- Peaks appearing **to the left of TMS** are said to be **downfield**
- The **further left** a peak appears, the **more deshielded** the carbon atom is

Important Points:

- Chemical shift values in **^{13}C-NMR are much larger** than in ^{1}H-NMR
- The chemical shift range of ^{13}C-NMR is approximately **0–220 ppm**
- The chemical shift depends on the **electronic environment** of the carbon atom

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Deduction of Molecular Structure Using ^{13}C-NMR

Each organic compound has a **unique ^{13}C-NMR spectrum**.
By:

- Counting the number of peaks
- Observing their chemical shift values
- Comparing them with standard reference data

we can determine the **types of carbon atoms present** in a molecule.

Key Structural Information Obtained:

- Different carbon environments (alkane, alkene, alkyne, aromatic, carbonyl, etc.)
- Symmetrical molecules show **fewer peaks** because identical carbons give a single signal

- Unsymmetrical molecules show **more peaks**

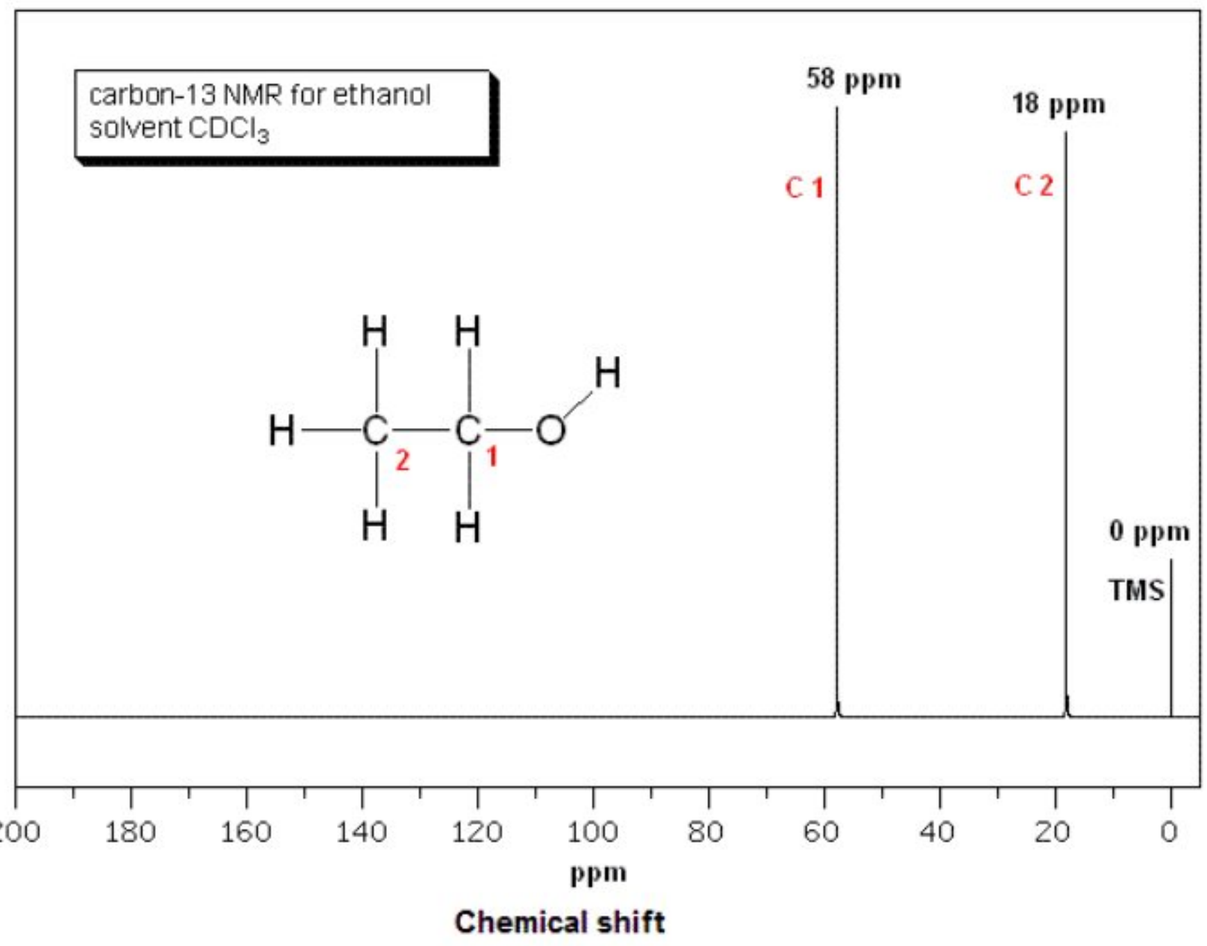
Approximate Chemical Shift Ranges in ^{13}C-NMR

Carbon Type	Chemical Shift (ppm)
Alkyl (C–C, C–H)	0–40
Carbon attached to heteroatom (O, N)	40–80
Alkyne (C≡C)	65–85
Alkene (C=C)	100–150
Aromatic carbon	110–160
Alcohol / Ether (C–O)	50–80
Aldehyde / Ketone (C=O)	190–220
Carboxylic acid / Ester	165–185
Amide	150–170

Example: ^{13}C-NMR Spectrum of Ethanol (C_2H_5OH)

Ethanol contains **two different carbon atoms**, so its ^{13}C-NMR spectrum shows **two peaks**.

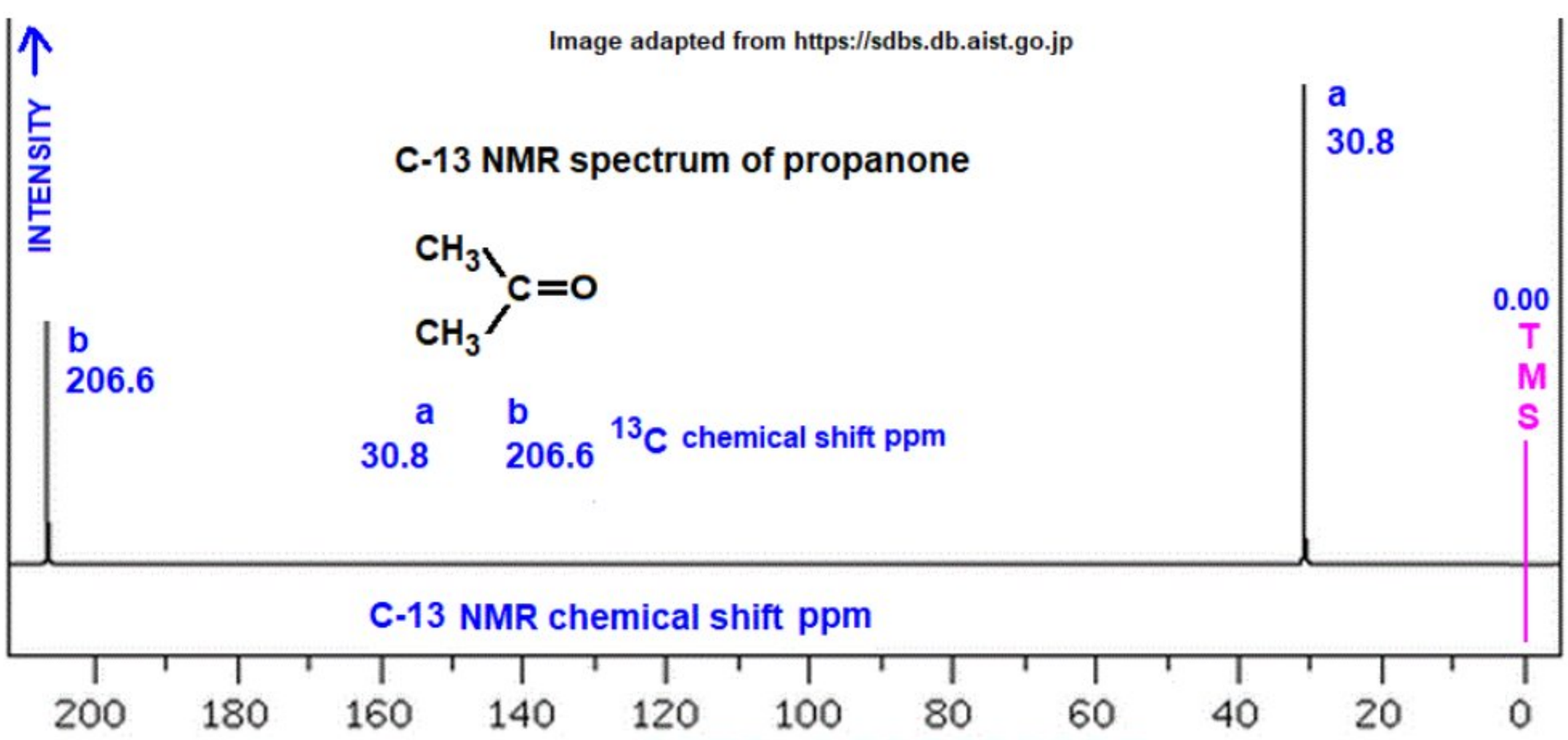
1. **Carbon attached to oxygen ($–CH_2–OH$)**
   - Strongly deshielded due to electronegative oxygen
   - Appears at ≈ **58 ppm**
2. **Methyl carbon ($–CH_3$)**
   - More shielded
   - Appears at ≈ **18 ppm**



Example: ^{13}C-NMR Spectrum of Acetone

Acetone ($CH_3–CO–CH_3$) contains three carbon atoms**, but its** ^{13}C-NMR spectrum shows only two peaks**.** This is because the two methyl ($–CH_3$) carbons are chemically identical due to the symmetrical structure of the molecule. Identical carbon atoms experience the same electronic environment and therefore produce only one signal**.**

- **Methyl carbons ($–CH_3$):**
  Both methyl carbons are equivalent and relatively well shielded. Their combined signal appears at **30.8 ppm**.
- **Carbonyl carbon (C=O):**
  The carbonyl carbon is strongly **deshielded** due to its double bond to the highly electronegative oxygen atom. As a result, it appears far downfield at **206 ppm**.



Key Principle of ^{13}C-NMR

In a ^{13}C-NMR spectrum**,** each unique carbon environment gives rise to a separate peak**.** Therefore, the number of peaks corresponds to the number of chemically different carbon atoms**,** not the total number of carbon atoms present in the molecule.

- Symmetrical molecules → **fewer peaks**
- Unsymmetrical molecules → **more peaks**

Steps to Predict the Number of Peaks in ^{13}C-NMR

In **^{13}C-NMR spectroscopy**, the number of peaks corresponds to the number of **chemically non-equivalent carbon atoms** in a molecule.

General Steps

1. **Look for symmetry in the molecule**
   Carbons that are symmetrical are **equivalent** and produce **only one peak**.
2. **Identify unique carbon environments**
   Carbons bonded to different atoms or having different bonding arrangements experience different electronic environments and give **separate peaks**.
3. **Ignore hydrogen count for peak number**
   In ^{13}C-NMR, peak number depends only on carbon environments, not on the number of hydrogens.

Example 1: Ethanol (C_2H_5OH)

Structure:
$CH_3–CH_2–OH$

Spectrum Analysis

- **Methyl carbon ($CH_3–$)**
  Bonded to three hydrogens and one carbon.
- **Methylene carbon ($–CH_2–$)**
  Bonded to two hydrogens, one carbon, and one oxygen.
- **Note:**
  Oxygen does not appear in the ^{13}C-NMR spectrum, but it affects the chemical shift of the attached carbon due to its high electronegativity.

Number of Unique Carbons

- Methyl carbon → **1 peak**
- Methylene carbon → **1 peak**

Expected Peaks: 2

Chemical Shift Positions

1. Methyl carbon: **10–20 ppm**
2. Methylene carbon: **50–60 ppm**

Example 2: Acetone (C_3H_6O)

Structure:
$(CH_3)_2CO$

Spectrum Analysis

- **Methyl carbons (CH_3):**
  Both methyl groups are equivalent because they are bonded to the same carbonyl carbon.
- **Carbonyl carbon (C=O):**
  Exists in a distinct environment due to the double bond with oxygen.

Number of Unique Carbons

- Methyl carbons → **1 peak**
- Carbonyl carbon → **1 peak**

Expected Peaks: 2

Chemical Shift Positions

1. Methyl carbons: **20–30 ppm**
2. Carbonyl carbon: **190–210 ppm**

Example 3: Butane (C_4H_{10})

Structure:
$CH_3–CH_2–CH_2–CH_3$

Spectrum Analysis

- **Methyl carbons (CH_3):**
  The two terminal methyl carbons are equivalent.
- **Methylene carbons (CH_2):**
  The two middle methylene carbons are equivalent.

Number of Unique Carbons

- Methyl carbons → **1 peak**
- Methylene carbons → **1 peak**

Expected Peaks: 2

Chemical Shift Positions

1. Methyl carbons: **10–20 ppm**
2. Methylene carbons: **20–40 ppm**

Example 4: Benzene (C_6H_6)

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Structure:
A six-membered aromatic ring

Spectrum Analysis

- All six carbons are equivalent due to the **high symmetry** of the benzene ring.

Number of Unique Carbons

- Aromatic carbons → **1 peak**

Expected Peaks: 1

Chemical Shift Position

- Aromatic carbon: **120–140 ppm**

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