



Module 10: Spectroscopy

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Module outline:

Introduction

Elementary ideas and simple applications of UV,

Visible, IR and ¹HNMR spectral Techniques

10.1. SPECTROSCOPY

It is a necessary tool, used for structure determination of organic molecule. Spectroscopy may be defined as the study of the quantized interaction of electromagnetic radiations with matter.

10.2. ELECTROMAGNETIC SPECTRUM

Electromagnetic spectrum covers a wide range of electromagnetic radiation from cosmic rays to radio waves. Electromagnetic radiation is radiant energy having the properties of both particles and waves.

A particle of electromagnetic radiation is called a *photon*. We may think of electromagnetic radiation as photons traveling at the speed of light. Because electromagnetic radiation has both particle-like and wave-like properties, it can be characterized by either its frequency (ν) or its wavelength (λ)

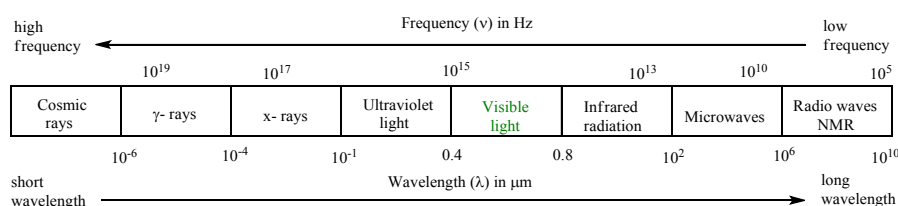
Frequency is defined as the number of wave crests that pass by a given point in one second. Frequency has units of hertz (Hz).

Wavelength is the distance from any point on one wave to the corresponding point on the next wave. Wavelength is generally measured in micrometers or nanometers. One micrometer (μm) is 10^{-6} of a meter; one nanometer (nm) is 10^{-9} of a meter.

The frequency of electromagnetic radiation, therefore, is equal to the speed of light (c) divided by the radiation's wavelength:

$$\nu = \frac{c}{\lambda} \quad c = 3 \times 10^{10} \text{ cm/s}$$

Short wavelengths have high frequencies, and long wavelengths have low frequencies.



The relationship between the energy (E) of a photon and the frequency (or the wavelength) of the electromagnetic radiation is described by the equation

$$E = h\nu = \frac{hc}{\lambda}$$

Where,

h = proportionality constant called *Planck's constant*, named after the German physicist who discovered the relationship.

c = velocity of light

λ = wavelength

Wave Number: It can be defined as the number of waves which can pass through per unit length in cm. It is reciprocal of wave length.

$$\gamma^- = \frac{1}{\lambda(\text{cm})}$$

10.3. ORIGIN OF ELECTRONIC SPECTRA

When electromagnetic radiations are passed through an organic compound, then some of wavelengths are absorbed while other remains unaffected. A molecule can only absorb radiation of certain frequency, if there exists within a molecule an energy difference of magnitude ΔE which is equal to $h\nu$. Suppose E_1 and E_2 are the two possible energy states of a system. The energy difference between the two states is given by ΔE .

$$\Delta E = E_2 - E_1$$

The energy transition from E_1 to E_2 or from E_2 to E_1 corresponds to the absorption or emission of energy exactly equivalent to the energy of the wavelength absorbed or emitted.

The absorbed or emitted energy is the form of electromagnetic radiation, the frequency of which is given by $\nu = \Delta E/h$ Hz

The energy change or the frequency of the electromagnetic radiation, emitted or absorbed can be recorded with the help of an instrument called *spectrometer*. Thus spectra so obtained can be broadly classified into two categories.

- i. **Emission Spectrum:** When there is a transition from a state of high energy to a stage of lower energy, the excess energy is emitted as a photon of energy $h\nu$ provided, $E = h\nu$. The spectrum recorded will be *emission spectrum*. Emission spectra are produced by heating a substance directly in a flame or heating it electrically and then passing the emitted radiation through a prism.
- ii. **Absorption Spectrum:** When there is a transition from a state of lower energy to a stage of higher energy, the energy absorbed will be exactly equal to the energy difference ΔE . The spectrum recorded will be *absorption spectrum*. UV, visible, IR and NMR spectra are examples of absorption spectra.

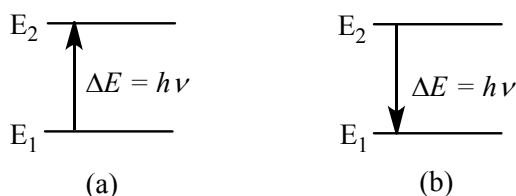


Fig. 10.1 Energy transition for the (a) absorption and (b) emission of electromagnetic radiation

Summary of Spectroscopic Techniques in Organic Chemistry

Spectroscopy	Radiation absorbed	Effects on the molecule
Ultraviolet (uv) visible	Uv-visible ($\lambda = 200-750$ nm)	Change in electronic energy levels within the molecule
Infrared (ir)	Infrared ($\lambda = 2.5-16$ μm)	Changes in the vibrational and rotational movements of the molecule
Nuclear magnetic resonance (nmr)	Radio ν , 60-500 MHz	Induces changes in the magnetic properties of certain atomic nuclei

10.4. ULTRAVIOLET & VISIBLE SPECTROSCOPY

U.V. and visible spectroscopy deals with the recording of the absorption of radiations in U.V. and visible region of electromagnetic spectrum. U.V. region extends from 10-400 nm. Since, U.V. and visible spectroscopy involves electronic transitions, so it is also called as "Electronic spectroscopy." It is used for elucidating nature of conjugated multiple bonds or aromatic rings.

10.5. LAMBERT – BEER'S LAW

Lambert's law states that the fraction of incident monochromatic radiation absorbed by a homogeneous medium is independent of the intensity of the incident radiation. Beer's law states that absorption of monochromatic radiation by a homogeneous medium is proportional to the number of absorbing molecules.

$$\log_{10} \frac{I_0}{I} = A = \epsilon cl$$

I_0 = Intensity of incident radiation

I = Intensity of radiation transmitted through sample solution.

A = Absorbance or optical density

ϵ = Molar extinction coefficient

c = conc. of solute in mole/litre

l = Path length of sample in cm.

The U.V. visible spectrophotometer records a U.V. or visible spectrum as a plot of wave length of absorbed radiation versus the intensity of absorption in terms of absorbance A or molar extinction coefficient.

Example 10.1. For a solution of camphor in hexane in a 10 cm cell, the absorbance A was found to be 2.52 at 295 nm with ϵ_{\max} 14. What is the concentration of camphor?

Solution:

$$A = \epsilon cl$$

$$A = 2.52, \epsilon = 14, l = 10 \text{ cm}$$

$$\therefore 2.52 = 14 \times c \times 10$$

$$c = \frac{14 \times 10}{2.52} = 1.8 \times 10^{-2} \text{ mole/litre}$$

10.6. ELECTRONIC TRANSITIONS

According to molecular orbital theory the excitation of molecule by absorption of radiation in U.V. and visible region involves promotion of electrons from a bonding or non-bonding orbital to antibonding orbitals. The following four types of electronic transition involves in U.V. visible regions:

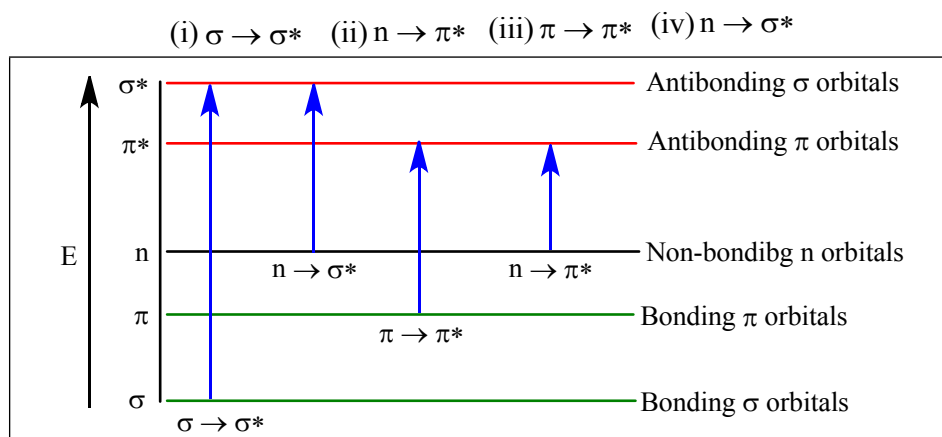
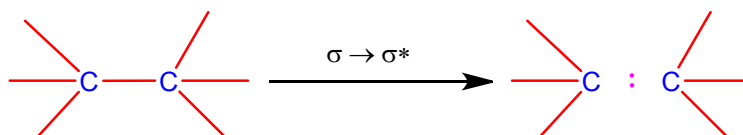


Fig. 10.2. Relative energies of electronic transitions

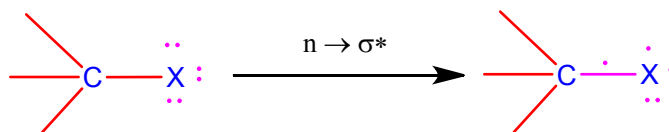
The usual order of energy required for various electronic transitions is

$$\sigma \rightarrow \sigma^* > n \rightarrow \sigma^* > \pi \rightarrow \pi^* > n \rightarrow \pi^*$$

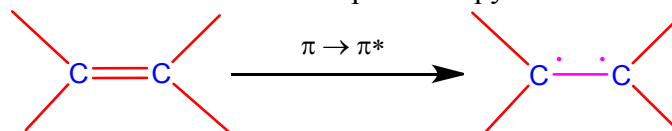
(i) **$\sigma \rightarrow \sigma^*$ Transition** : The promotion of an electron from sigma bonding orbital to antibonding sigma orbital is called as $\sigma \rightarrow \sigma^*$ transition. It occurs at high energy level since σ bonds are very strong in nature. Example: alkanes only.



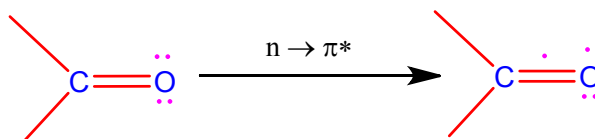
(ii) **$n \rightarrow \sigma^*$ Transition**: The promotion of an electron from nonbonding orbital to antibonding sigma orbital is called as $n \rightarrow \sigma^*$ transition. Example: Alkyl Halide, Alcohols etc.



(iii) **$\pi \rightarrow \pi^*$ Transition**: The promotion of an electron from pi bonding orbital to pi antibonding orbital is called as $\pi \rightarrow \pi^*$ transition. It requires lower energy. Example: Alkene, Alkynes



(iv). $n \rightarrow \pi^*$ **Transition:** The promotion of an electron from a non-bonding orbital to pi antibonding orbital is called as $n \rightarrow \pi^*$ transition. It occurs at lowest energy. Example: Carbonyl compounds, nitriles etc.



10.7. CHROMOPHORE

A covalently unsaturated group responsible for absorption in the U.V. or visible region is known as a chromophore. For example: $C=C$, $C \equiv C$, $C=O$, $C \equiv C$, $C=C$, $C=O$, $C \equiv N$, $C \equiv N$, $N \equiv N$, NO_2 etc. If a compound absorbs light in the visible region (400-800 nm), only then it appears coloured. Thus, a *chromophore* may or may not impart colour to a compound depending on whether the chromophore absorbs radiation in the visible or UV region.

Chromophores like $C=C$ or $C \equiv C$ having π electrons undergo $\pi \rightarrow \pi^*$ transitions and those having both π and non-bonding electrons, e.g. $C=O$, $C \equiv N$, $C=O$ or $N \equiv N$, undergo $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ and $n \rightarrow \sigma^*$ transitions. Since the wavelength and intensity of absorption depend on the number of factors, there are no set rule for the identification of a chromophore.

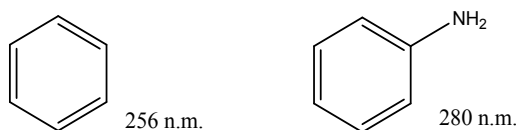
10.8. AUXOCHROME

A covalently saturated group which, when attached to chromophore, changes both the wave length and intensity of the absorption maximum is known as *auxochrome*, e.g. NH_2 , OH , SH , NH_2 , OH , SH , halogens etc. Auxochrome generally increase the value of λ_{max} as well as ϵ_{max} by extending the conjugation through resonance. These are also called *colour enhancing group*. An auxochrome itself does not show absorption above 200 nm. Actually, the combination of chromophore and auxochrome behaves as a new chromophore having different value of λ_{max} and ϵ_{max} . For example, benzene shows λ_{max} 256 nm, ϵ_{max} 200, whereas aniline shows λ_{max} 280 nm, ϵ_{max} 1430 (both increased). Hence, NH_2 group is an auxochrome which extends the conjugation involving the lone pair of electrons on the nitrogen atom resulting in the increased values of λ_{max} and ϵ_{max} .

10.9. ABSORPTION AND INTENSITY SHIFTS

10.9.1. Bathochromic Shift

The shift of an absorption maximum to a longer wave length due to the presence of auxochrome is called as Bathochromic shift or “Red shift.”



10.9.2. Hypsochromic Shift

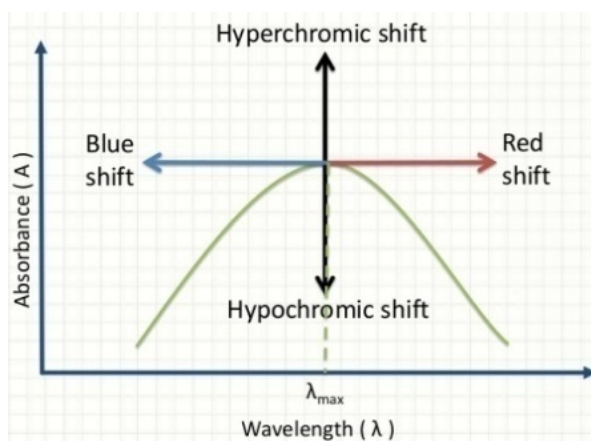
The shift of an absorption maximum to shorter wave length is called as Hypsochromic shift or Blue shift. It is due the loss of conjugation.

10.9.3. Hyperchromic Effect

An effect, which leads to an increases absorption intensity is called as “Hyperchromic Effect.”

10.9.4. Hypochromic Effect

An effect which leads to a decrease in absorption intensity is called as “Hypochromic Effect.”



10.10. Applications of Ultraviolet and Visible Spectroscopy

Some important applications of UV and visible spectroscopy to organic chemistry are summarised as follows.

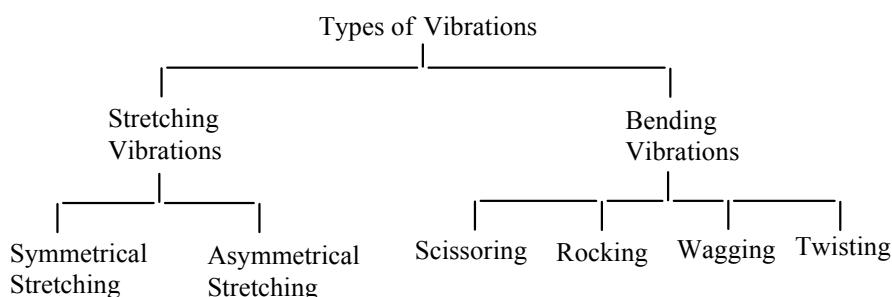
1. Detection of functional group (Chromophore).
2. Detection of conjugation and elucidation of its nature.
3. Study of extent of conjugation.
4. Distinction between conjugated and unconjugated compounds.
5. Study of steric strain.
6. Determination of configurations of geometrical isomers.
7. Study of tautomerism
8. Confirmation of suspected phenols and aromatic amines.
9. Study of structural features in different solvents.

10.11. INFRARED (IR) SPECTROSCOPY

Infrared spectroscopy allows us to determine the kinds of functional groups a compound has. It deals with the recording of the absorption of radiations in the infra red region of the electromagnetic spectrum. The position of a given infrared absorption is expressed in terms of wave number ($\bar{\nu}$) ($\bar{\nu}$). The infrared region is 2.1 -15 or 4000-667 cm^{-1} is of greatest practical use to organic chemist.

The absorption of infrared radiation by a molecule occurs due to quantized vibrational and rotational energy changes, so it is also called as vibrational– rotational spectra.

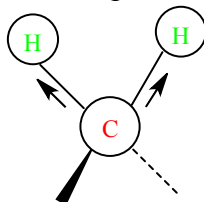
10.12. TYPES OF VIBRATIONS



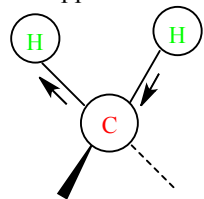
10.12.1. Stretching vibrations

In this type of vibrations, the distance between two atoms increases or decreases but the atoms remains in the same bond axis. It is of two types:

(a). Symmetrical Stretching: In this mode of vibration the movement of atoms with respect to common central atom is simultaneously in the same direction along the same bond axis.



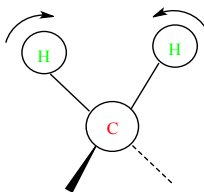
(b). Asymmetrical Stretching: In this vibration, one atom approaches the central atom while other departs from it.



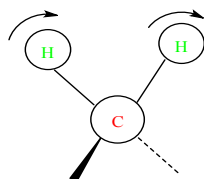
10.12.2. Bending Vibrations

In this type of vibrations the positions of the atoms change with respect to their original bond axis. It is of four types:

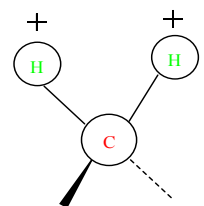
(a). Scissoring: In this mode of vibrations the movement of atoms is in the opposite directions with change in their bond axis as well as bond angle they form with central atom.



(b). Rocking: In this vibration the movement to atom takes place in the same directions with change in their bond axis.



(c). Wagging: In this vibration two atoms simultaneously move above and below the plane with respect to central atom.



(d). Twisting: In this mode of vibration one of the atom moves up and the other moves down the plane with respect to central atom.

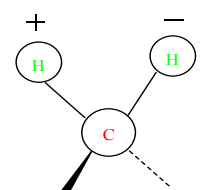



Table 10.1 Important Infrared Stretching Frequencies

Type of Bond	γ^- (cm ⁻¹)
C \equiv N	2260-2220
C \equiv C	2260-2100
C=C	1680-1600
C=N	1650-1550
	1600, 1500-1430
C=O	1780-1650
C—O	1250-1050
C—N	1230-1020
O-H (alcohol)	3650-3200
O-H (carboxylic acid)	3300-2500
N-H	3500-3300
C-H	3300-2700

10.13. NUMBER OF FUNDAMENTAL VIBRATIONS

In case of a non-linear molecule, three of the degrees of freedom describe rotation and three describe translation. Thus, the remaining ($3n - 3 - 3$) = $3n - 6$ degrees of freedom are its vibrational degrees of freedom of fundamental vibrations, because

Total degrees of freedom ($3n$) = Translation + Rotational + Vibrational degrees of freedom

Example: A non-linear molecule ethane (C₂H₆), the vibrational degree of freedom can be calculated as:

Number of atoms (n) = 8

Total degrees of freedom ($3n$) = $3 \times 8 = 24$

Rotational degrees of freedom = 3

Translational degrees of freedom = 3

Therefore, vibrational degrees of freedom = $24 - 3 - 3 = 18$

Thus, theoretically there should be 18 absorption bands in the IR spectrum of ethane.

Example: In case of benzene (C₆H₆), the number of vibrational degrees of freedom can be calculated as follows:

Number of atoms (n) = 12

Total degrees of freedom ($3n$) = $3 \times 12 = 36$

Rotational degrees of freedom = 3

Translational degrees of freedom = 3

Therefore, vibrational degrees of freedom = $36 - 3 - 3 = 30$

Thus, theoretically there should be 30 absorption bands in the IR spectrum of benzene.

In case of linear molecule, only two degrees of freedom describe rotation and three describe translation. Thus, the remaining ($3n - 2 - 3$) = $3n - 5$ degrees of freedom are vibrational degrees of freedom or fundamental vibrations.

Example: The number of vibrational degrees of freedom for the linear carbon dioxide molecule can be calculated as follows:

Number of atoms (n) = 3

Total degrees of freedom ($3n$) = $3 \times 3 = 9$

Rotational degrees of freedom = 2

Translational degrees of freedom = 3

Therefore, vibrational degrees of freedom = $9 - 2 - 3 = 4$

Since, each vibrational degree of freedom correspond to a fundamental vibration and each fundamental vibration correspond to an absorption band, for carbon dioxide molecule there should be four theoretical fundamental bands.

10.14. FINGER PRINT REGION

I. R. spectrum covers a wide range from 4000-667 cm⁻¹. It can be divided into two regions i.e. 4000-1400 cm⁻¹, it is the region where most of the functional groups shows absorption bands, it is called as functional group region. The region from 1400-667 cm⁻¹ is called as **finger print region**. The overall pattern in the finger print region is characteristic of compound as a whole

because each compound shows a unique pattern in this region. So, compounds can be effectively identified by comparing their finger print region.

10.15. APPLICATIONS OF INFRARED SPECTROSCOPY

Some important applications of UV and visible spectroscopy to organic chemistry are summarised as follows.

1. Detection of functional groups.
2. Confirmation of the identity of compounds.
3. Estimation of the purity of samples.
4. Study of hydrogen bonding.
5. Calculation of force constants.
6. Determination of orientations in aromatic compounds.
7. Study of the progress of reactions.

10.16. PROTON NUCLEAR MAGNETIC RESONANCE (PMR OR ^1H NMR) SPECTROSCOPY

NMR spectroscopy involves nuclear magnetic resonances which depend on the magnetic property of atomic nuclei. Thus NMR spectroscopy deals with nuclear magnetic transitions between magnetic energy levels of the nuclei in molecules. NMR signals were first observed in 1945 independently by Prucell at Harvard and Bloch at Stanford. The first application of NMR to the study of structure was made in 1951 and ethanol was the first compound thus studied. In 1952, Prucell and Bloch won the Nobel Prize in Physics for their discovery.

NMR spectroscopy helps to identify carbon-hydrogen framework of an organic compound. The hydrogen nuclei were the first nuclei, studied by nuclear magnetic resonance hence acronym NMR is generally mean to ^1H NMR. It operates at radio frequency (R.F) region.

Certain nuclei have allowed spin states of $+1/2$ and $-1/2$ and this property allows them to be studied by NMR. Examples of such nuclei are ^1H , ^{13}C , ^{15}N , ^{19}F , ^{31}P .

10.17. INSTRUMENTATION

NMR signals are detected by spectrometers. The NMR spectrometer detects the signals and displays them as a plot of signal frequency versus intensity. The term nuclear magnetic resonance comes from the fact that the nuclei are in resonance with radiofrequency radiation.

The schematic diagram of a NMR spectrometer containing the following components is given in Fig. 10.3.

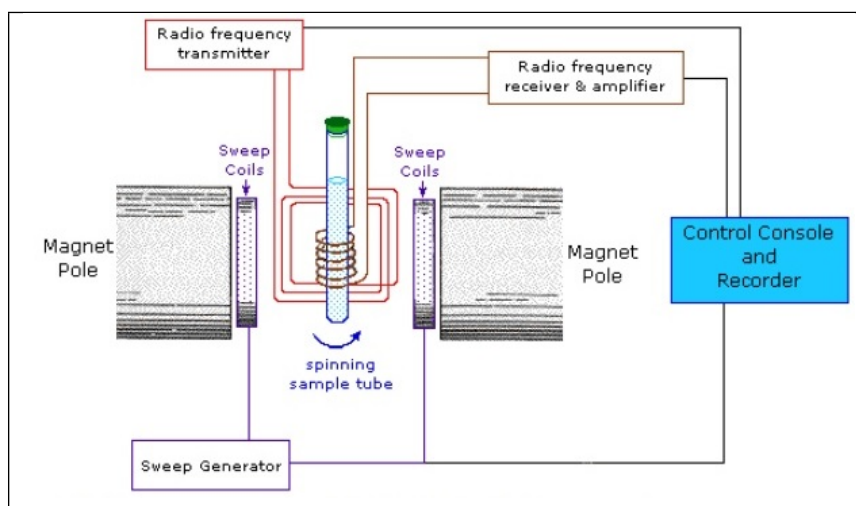


Fig. 10.3 Schematic diagram of a NMR spectrometer

10.18. SHIELDING AND DESHIELDING

Under the influence of applied magnetic field, electrons surrounding a nucleus start to circulate perpendicular to the applied magnetic field (H_0), and so they generate a secondary magnetic field called *induced magnetic field* (σH_0) which oppose the applied magnetic field (H_0) in the region of the nucleus, e.g. proton. Thus, the nucleus experiences a weaker magnetic field (H_{eff})

than the applied magnetic field (H_0), and it is said to be *shielded*. This type of shielding is termed diamagnetic shielding and its effect is termed as *shielding effects*, i.e.

$$H_{eff} = H_0 - \sigma H_0$$

Where σ is screening or shielding constant.

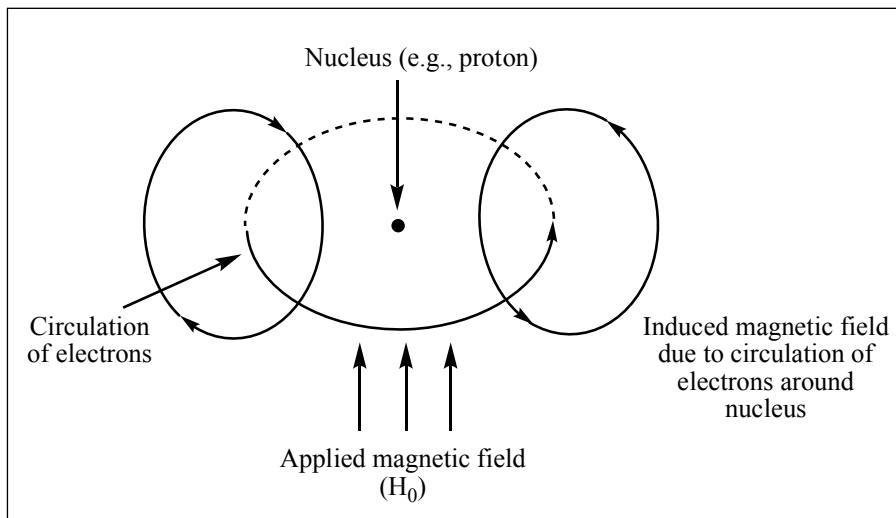


Fig. 10.4 Diamagnetic shielding of nucleus by circulating electrons

If the induced field reinforces the applied field, then the field experienced by the proton is greater than the applied field. Such a proton is said to be deshielded and this effect is termed as *deshielding effect*.

Compared to a naked proton, a shielded proton requires higher field strength, whereas deshielded proton requires lower field strength for transition. Thus, shielding shifts the absorption position upfield, whereas deshielding shifts the absorption position downfield and these effects are termed as shielding and deshielding effects, respectively.

At 300 MHz, an unshielded naked proton absorbs at 70,459 gauss. But a shielded proton requires a stronger field. For example, if a proton is shielded by 1 gauss when the external field is 70,459, the effective magnetic field experienced by the proton is 70,458 gauss. At this field proton will not absorb energy by flipping. If the external field is increased to 70,460 gauss, the effective magnetic field experienced by the proton will be 70,459 (70,460 - 1 = 70,459). At this field proton will absorb energy which brings this proton into resonance.

Thus, magnetic field must be increased slightly (in comparison to naked proton) above 70,459 gauss (at 300 MHz) for resonance of a shielded proton.

If all protons were shielded by the same amount, they would all be in resonance at the same combination of frequency and magnetic field. Fortunately protons in different chemical environments are shielded by different amounts. Magnitude of shielding depends on the electron density around proton. The higher the electron density around the proton, the higher is the shielding and thus higher is the field needed for flipping. For example CH_3 protons of $\text{CH}_3\text{-Cl}$ is more shielded than CH_3F because electronegativity of fluorine is more than the chlorine. Thus CH_3 protons of CH_3F absorbs at lower field than the CH_3 protons of CH_3Cl .

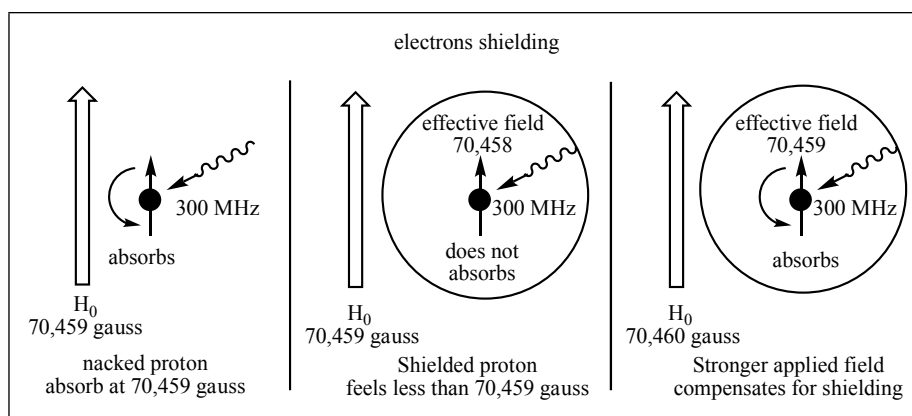
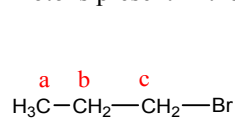


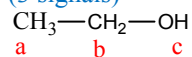
Fig. 10.5 Shielded protons

10.19. NUMBER OF SIGNALS IN ^1H NMR SPECTRUM

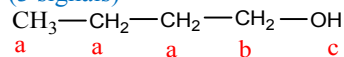
Protons present in the same environment are chemically equivalent protons and will give same signal.



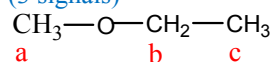
(3 signals)



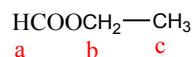
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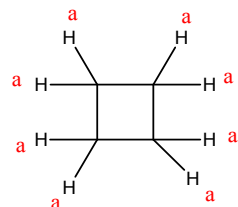
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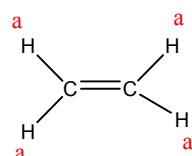
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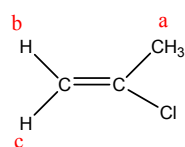
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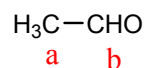
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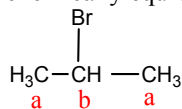
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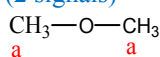
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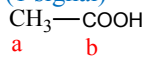
(2 signals)



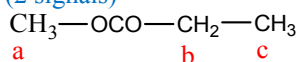
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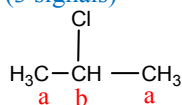
(1 signal)



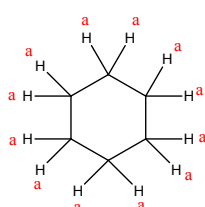
(2 signals)



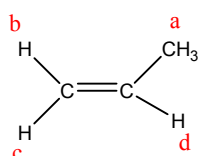
(3 signals)



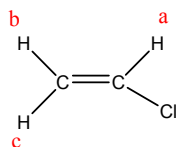
(2 signals)



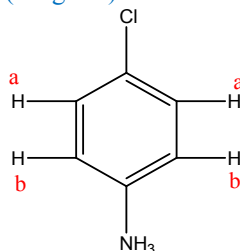
(1 signal)



(4 signals)



(3 signals)



(2 signals)

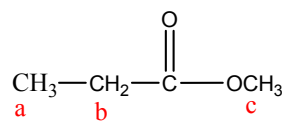
10.20. SPLITTING OF THE SIGNALS

Splitting is caused by protons bonded to adjacent (i.e., directly attached) carbons. The splitting of a signal is described by ($n+1$) **rule**, where N is the number of *equivalent* protons bonded to *adjacent* carbons. By “**equivalent protons**,” we mean that the protons bonded to an adjacent carbon are equivalent to each other, but not equivalent to the proton giving rise to the signal.

Keep in mind that it is not the number of protons giving rise to a signal that determines the multiplicity of the signal; rather, it is the number of protons bonded to the immediately adjacent carbons that determines the multiplicity.

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For example, the signal for the **a** protons in the following compound will be split into three peaks (a triplet) because the adjacent carbon is bonded to two hydrogens. The signal for the **b** protons will appear as a quartet because the adjacent carbon is bonded to three hydrogens, and the signal for the **c** protons will be a singlet.



Multiplicity of the signals

Number of equivalent proton causing splitting	Multiplicity of the signal
0	Singlet
1	Doublet
2	Triplet
3	Quartet
4	Quartet
5	Sextet
6	Septet

10.21. CHEMICAL SHIFT

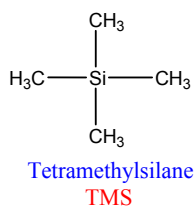
Shielding and deshielding shifts in the NMR absorption position are called *chemical shifts* because they arise from the circulation of electrons in chemical bonds. The chemical shift indicates how far the signal is from the TMS peak. The most common scale for chemical shift is δ scale. TMS is assigned at zero position on δ scale.

$$\delta = \text{chemical shift (ppm)} = \frac{\text{distance downfield from TMS (Hz)}}{\text{operating frequency of the spectrometer (MHz)}}$$

Most proton chemical shifts fall in the range from 0 to 10 ppm.

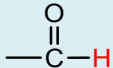
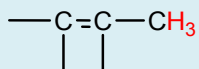
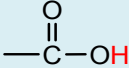
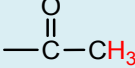
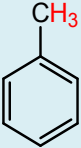
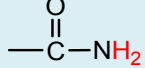
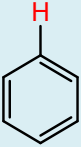
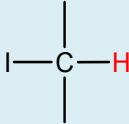
10.22. TMS (TETRA METHYL SILANE)

It is used as reference compound in NMR spectroscopy. It is highly volatile in nature. The methyl protons of TMS are in a more electron-dense environment than are most protons in organic molecules, because silicon is less electronegative than carbon. Consequently, the signal for the methyl protons of TMS is at a lower frequency than most other signals (i.e., it appears at 0 ppm value on δ scale).



10.23. COUPLING CONSTANT

The distance, in hertz, between two adjacent peaks of a split NMR signal is called the **coupling constant** (denoted by **J**). The coupling constant for **H_a** being split by **H_b** is denoted by **J_{ab}**. The signals of coupled protons (protons that split each other's signal) have the same coupling constant; in other words, **J_{ab} = J_{ba}**. Coupling constants are useful in analyzing complex NMR spectra because protons on adjacent carbons can be identified by identical coupling constants.

Type of proton	Approximate chemical shift (δ ppm)	Type of proton	Approximate chemical shift (δ ppm)
(CH ₃) ₄ Si	0		9-10
-CH ₃	0.9	RNH ₂	1.5-4
-CH ₂ - -CH-	1.3 1.4	ROH ArOH	2-5 4-7
	1.7		10-12
 	2.1 2.3	 R-O-CH ₃	5-8 3.3
	6.5-8		2.4-5

10.24. APPLICATIONS OF NMR SPECTROSCOPY

1. Identification of structural isomers.
2. Detection of aromaticity.
3. Detection of hydrogen bonding.
4. Distinction between cis-trans isomers and conformers.
5. Detection of partial double bond character.
6. Quantitative analysis.
7. **Magnetic Resonance Imaging**

NMR has become an important tool in medical diagnosis because it allows physicians to probe internal organs and structures without invasive surgical methods or the harmful ionizing radiation of X-rays. When NMR was first introduced into clinical practice in 1981, the selection of an appropriate name was a matter of some debate. Because some members of the public associate nuclear processes with harmful radiation, the "N" was dropped from the medical application of NMR, now known as **magnetic resonance imaging (MRI)**. The spectrometer is called an **MRI scanner**. MRI scans, therefore, can sometimes provide much more information than images obtained by other means. *The 1991 Nobel Prize in chemistry was awarded to **Richard R. Ernst** for two important contributions: FT-NMR spectroscopy and an NMR tomography method that forms the basis of magnetic resonance imaging (MRI).*

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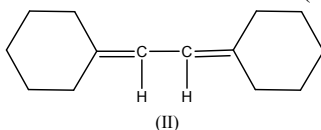
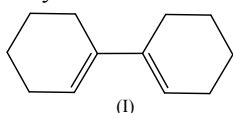
Vishal Srivastava is working as Assistant Professor, Department of Chemistry, C.M.P. College, (Constituent P.G. College of Central University of Allahabad) Prayagraj, India. He has completed Graduation (B.Sc.), Post-Graduation (M.Sc.) in Organic Chemistry and Doctoral Degree (D.Phil.) from Department of Chemistry, University of Allahabad, India. His current research work involves the designing of novel biologically active photoredox catalysed synthetic organic compounds.

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2. P. C. Jain (2015) "Engineering Chemistry" Dhanpat Rai Publishing Company.
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EXERCISE

1. Why β -carotene absorbs light in visible region.
2. What are auxochromes. Why and how auxochrome increases colouring power of chromophore?
3. Discuss the types of electronic transition in UV – visible spectroscopy.
4. Define the term Chromophore and Auxochrome in UV spectroscopy.
5. Why λ_{\max} for the diene(I) is observed at a lower n.m. than (II)?



6. For a XY_2XY_2 bent molecule show various types of stretching and bending vibrations in I.R.?
7. What is the importance of finger print region I.R. spectroscopy?
8. Two isomers A and B of molecular formula C_3H_6O gives I.R. absorption band at 1650 cm^{-1} and 1710 cm^{-1} respectively. Assign structural formula to isomers A and B?
9. An organic compound of molecular formula C_7H_6O shows absorption peaks at $3010, 2700, 1600, 1580, 1520, 1480$ and 1270 cm^{-1} in its I.R. spectrum. Suggest its structure.
10. How will you distinguish between the following pairs of compounds on the basis of infrared spectroscopy?
 - (i). CH_3COOH and $CH_3COOC_2H_5$
 - (ii). C_2H_5OH and $C_2H_5OC_2H_5$
11. Why TMS is used as standard reference in NMR spectroscopy?
12. How many NMR signals are obtained in $CH_3CHOHCH_2CH_3$?
13. What is shielding and deshielding?
14. How many NMR signals would you expect in the NMR spectra of the following compound: Chlorobutane, 2-Chlorobutane, Cyclohexane, n-Butanol and Acetic acid.
15. How many NMR signals are obtained in 2-Bromopropane?
16. How many NMR signals are obtained in Cyclobutane and 2-Chloropropane?
17. Show the number of expected 1H NMR signals and their splitting pattern in $CH_3OCOCH_2CH_3$ and $HCOOCH_2CH_3$?
18. What are equivalent and non equivalent protons in NMR spectroscopy? A compound having molecular formula C_4H_9Br gave the following set of 1H NMR signals: $\delta 1.04$ (6H, d); $\delta 1.95$ (1H, m) and $\delta 3.33$ (2H, d). Giving proper reasons suggest a structure consistent with the above data.