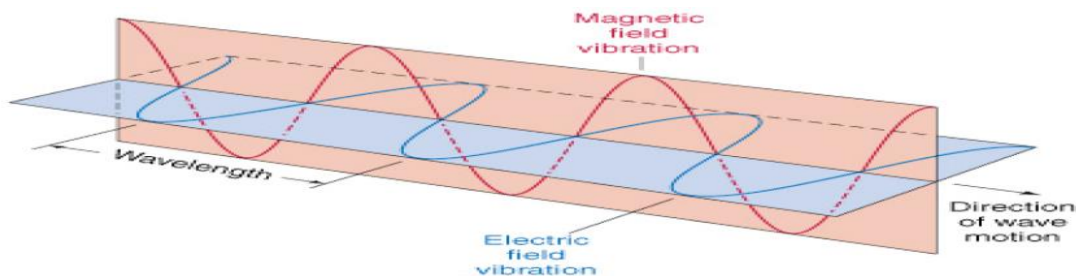


INTRODUCTION TO SPECTROSCOPY

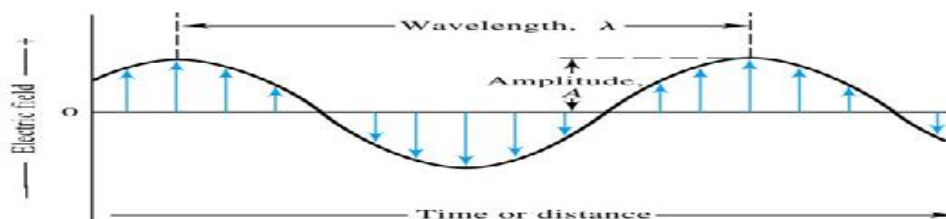
Spectroscopy is a method of analysis based on the interaction, absorption (or) production of light by matter. (Also may include the interaction of electrons, ions or acoustics with matter)



TERMS IN ELECTRO MAGNETIC RADIATION

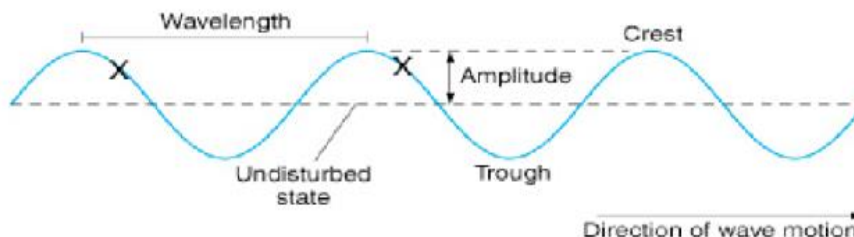
1) Amplitude (A):

- Amplitude is the distance from the maximum vertical displacement of the wave to the middle of the wave.
- This measures the magnitude of oscillation of a particular wave. In short, the amplitude is basically the height of the wave.



2) Wavelength (λ):

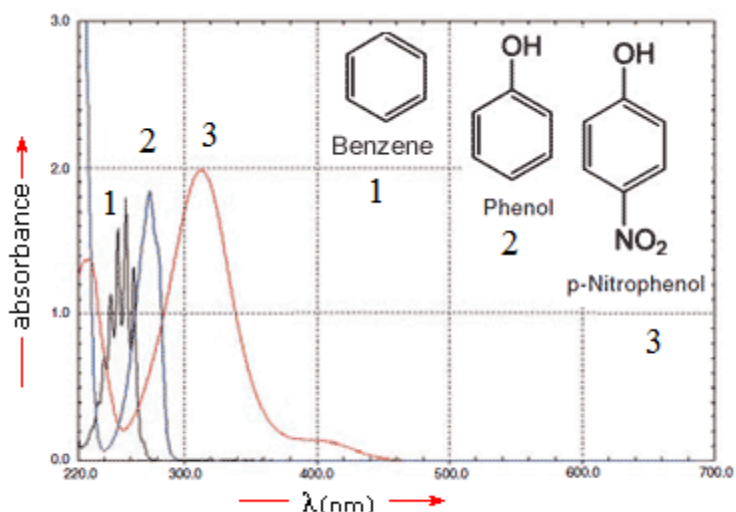
- Wavelength is the distance of one full cycle of the oscillation.
- Longer wavelength waves such as radio waves carry low energy; this is why we can listen to the radio without any harmful consequences.
- Shorter wavelength waves such as x-rays carry higher energy that can be hazardous to our health. Consequently lead aprons are worn to protect our bodies from harmful radiation when we undergo x-rays.
- Units: Distance (nm, cm and m) from peak to peak.



INTRODUCTION TO UV SPECTROSCOPY

UV spectroscopy is an important tool in analytical chemistry. The other name of UV (Ultra-Violet) spectroscopy is Electronic spectroscopy, as it involves the promotion of the electrons from the ground state to the higher energy or excited state.

UV spectroscopy is type of absorption spectroscopy in which light of ultra-violet region (200-400 nm.) is absorbed by the molecule. Absorption of the ultra-violet radiations results in the excitation of the electrons from the ground state to higher energy state.



Absorption Spectra of Benzene, Phenol, and p-Nitrophenol

Class	transition	Wavelength (nm) max
R-OH	$n \rightarrow \sigma^*$	180
R-O-R	$n \rightarrow \sigma^*$	180
R-NH ₂	$n \rightarrow \sigma^*$	190
R-SH	$n \rightarrow \sigma^*$	210
R ₂ C=CR ₂	$\pi \rightarrow \pi^*$	175
R-C≡C-R	$\pi \rightarrow \pi^*$	170

PRINCIPLE OF UV SPECTROSCOPY

UV spectroscopy obeys the Beer-Lambert law, which states that:

When a beam of monochromatic light is passed through a solution of an absorbing substance, the rate of decrease of intensity of radiation with thickness of the absorbing solution is proportional to the incident radiation as well as the concentration of the solution.

The expression of Beer-Lambert law is: $A = \log (I_0/I) = Ecl$

A = absorbance

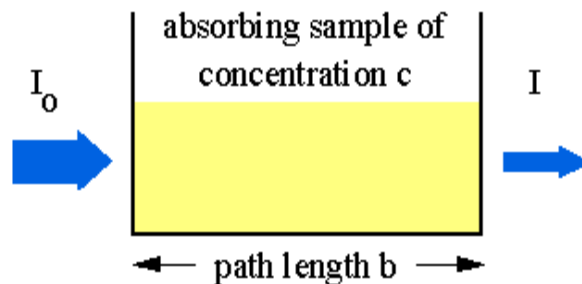
I₀ = intensity of light incident upon sample cell

I = intensity of light leaving sample cell

C = molar concentration of solute

L = length of sample cell (cm)

E = molar absorptivity.



From the Beer-Lambert law it is clear that greater the number of molecules capable of absorbing light of a given wavelength, the greater the extent of light absorption. This is the basic principle of UV spectroscopy.

INSTRUMENTATION AND WORKING OF UV SPECTROSCOPY

Instrumentation and working of the UV spectrometers can be studied simultaneously. Most of the modern UV spectrometers consist of the following parts:

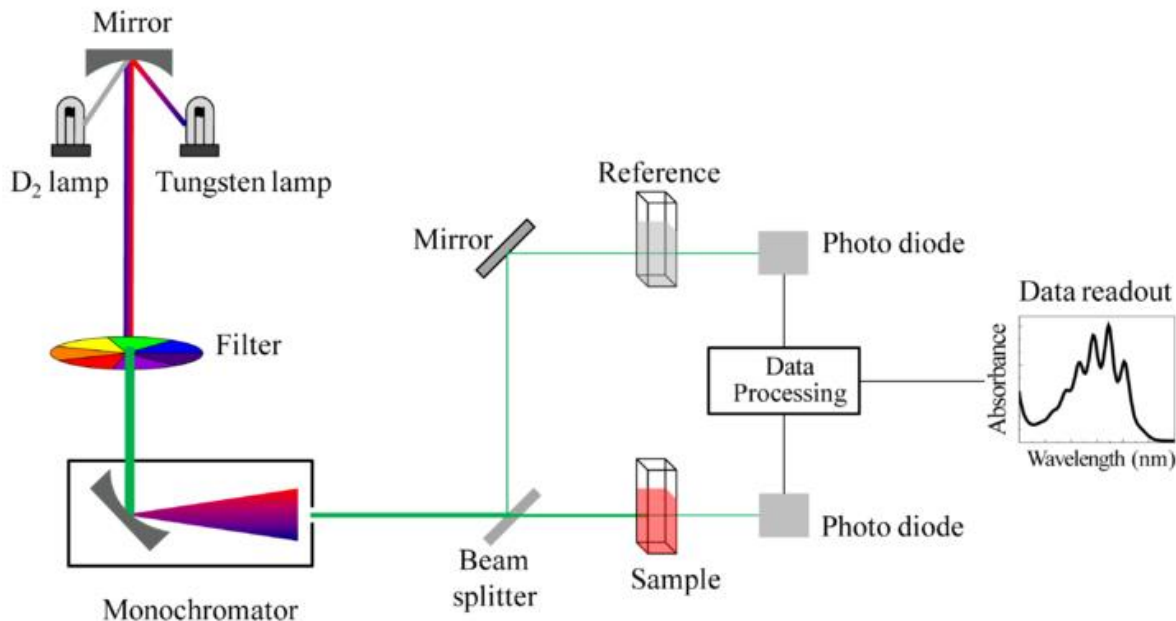
1. Light Source: Tungsten filament lamps and Hydrogen-Deuterium lamps are most widely used and suitable light source as they cover the whole UV region. Tungsten filament lamps are rich in red radiations. More specifically they emit the radiations of 375 nm, while the intensity of Hydrogen-Deuterium lamps falls below 375 nm.

2. Monochromator: Monochromators generally composed of prisms and slits. The most of the spectrophotometers are **double beam spectrophotometers**. The radiation emitted from the primary source is dispersed with the help of rotating prisms. The various wavelengths of the light source which are separated by the prism are then selected by the slits such the rotation of the prism results in a series of continuously increasing wavelength to pass through the slits for recording purpose. The beam selected by the slit is monochromatic and further divided into two beams with the help of another prism.

3. Sample and reference cells: One of the two divided beams is passed through the sample solution and second beam is passed through the reference solution. Both sample and reference solution are contained in the cells.

These cells are made of either silica or quartz. Glass can't be used for the cells as it also absorbs light in the UV region.

4. Detector: Generally two photocells serve the purpose of detector in UV spectroscopy. One of the photocell receives the beam from sample cell and second detector receives the beam from the



reference. The intensity of the radiation from the reference cell is stronger than the beam of sample cell. This results in the generation of pulsating or alternating currents in the photocells.

5. Recording devices: Most of the time amplifier is coupled to a pen recorder which is connected to the computer. Computer stores all the data generated and produces the spectrum of the desired compound.

SELECTION RULES OF UV SPECTROSCOPY

1. Laporte selection rule: There must be a change in the symmetry of the complex Electric dipole transition can occur only between states of opposite symmetry.

Laporte-allowed transitions: $g \rightarrow u$ (or) $u \rightarrow g$

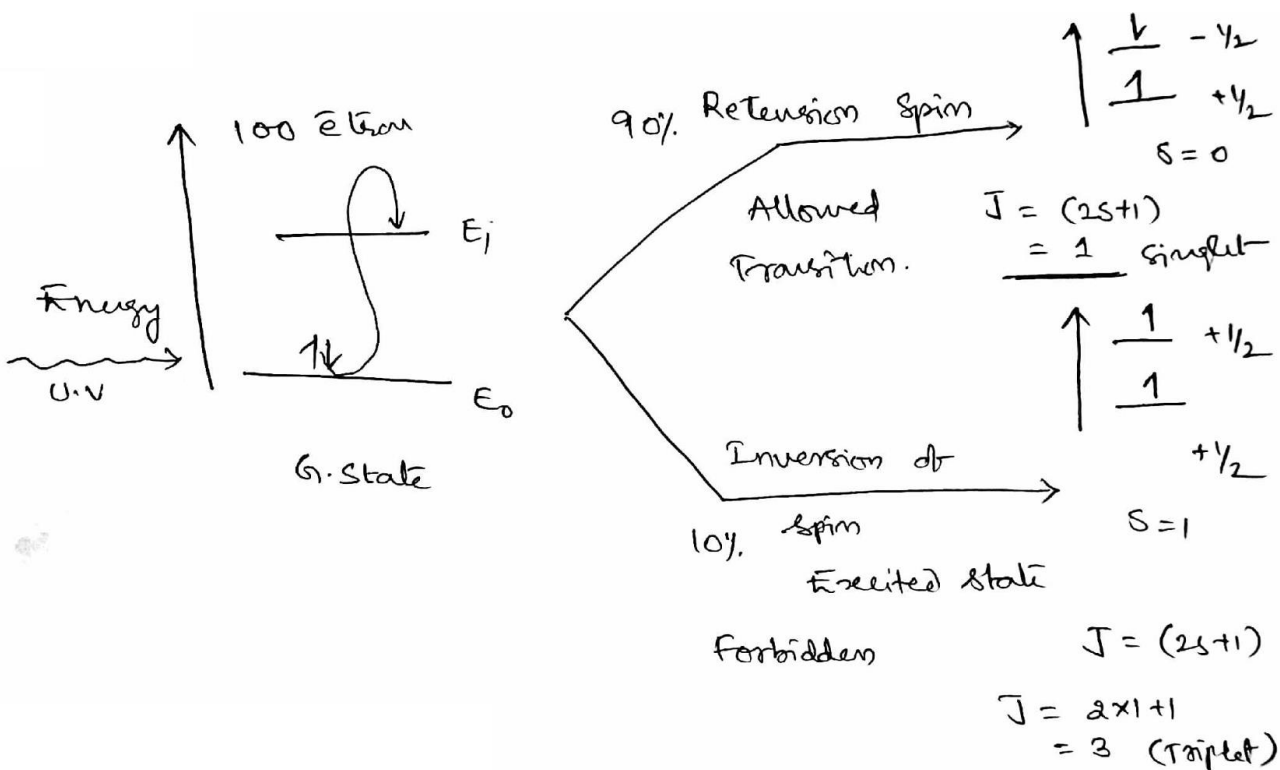
Laporte-forbidden transitions: $g \rightarrow g$ (or) $u \rightarrow u$

‘g’ stands for gerade – compound with a center of symmetry, ‘u’ stands for ungerade – compound without a center of symmetry.

2. Spin Selection Rule: The overall spin 'S' of a complex must not change during an electronic transition, hence, $\Delta S = 0$.

$$J = [2S+1] \quad \text{where, } J = \text{spin multiplicity, } S = \text{electron spin}$$

Electron transitions with retention of spin orientation is allowed, with inversion of spin orientation is Forbidden transition this is known as spin exclusion principle.

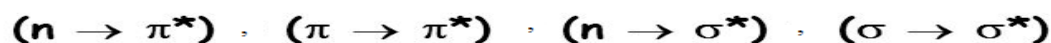


Electron transitions with retention of spin multiplicity are allowed transition. Electron transitions with inversion of spin multiplicity are forbidden transition.

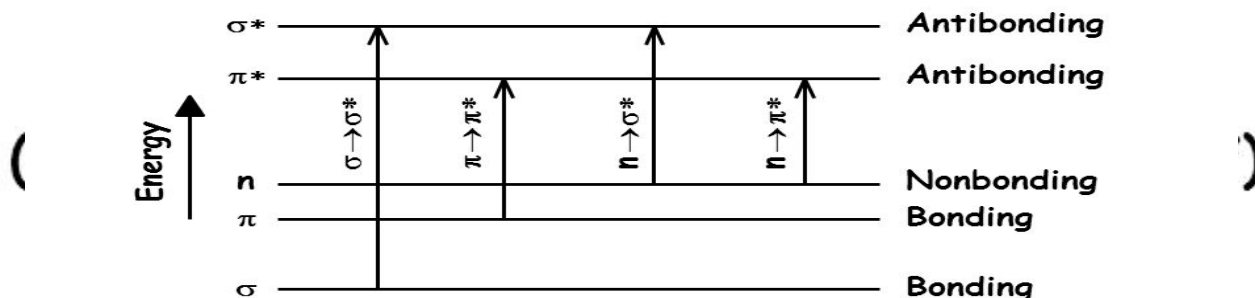
3. Selection rule based on transition from HOMO to LUMO:

- Generally, the most favoured transition is from the highest occupied molecular orbital (HOMO) to lowest unoccupied molecular orbital (LUMO).
- For most of the molecules, the lowest energy occupied molecular orbitals are **s orbital**, which correspond to **sigma bonds**. The **p orbitals** are at somewhat higher energy levels, the orbitals (nonbonding orbitals) with unshared paired of electrons lie at higher energy levels.
- The unoccupied or antibonding orbitals (π^* and σ^*) are the highest energy occupied orbitals. In all the compounds (other than alkanes), the electrons undergo various transitions.

- Some of the important transitions with increasing energies are:



**Bonding electrons appear in σ and π molecular orbitals
nonbonding in n**



**Electronic transitions can occur between various states.
The energy of the transitions increases in the following order:**



CONCEPT OF CHROMOPHORE AND AUXOCHROME IN THE UV SPECTROSCOPY

1. Chromophore is defined as any isolated covalently bonded group that shows a characteristic absorption in the **ultraviolet or visible region (200-800 nm)**. Chromophores can be divided into two groups:

a. Chromophores which contain **π electrons** and which undergo **π - π^*** transitions.

Ex: Ethylenes and acetylenes

b. Chromophores which contain both **π - electrons and n (non-bonding) electrons** undergo two types of transitions: **π - π^* and n - π^*** .

Ex: Carbonyl, nitriles, azo compounds, nitro compounds etc.

2. Auxochromes: An auxochrome can be defined as any group which does not itself act as a chromophore but whose presence brings about a shift of the absorption band towards the longer wavelength of the spectrum.

Ex: -OH, -OR, -NH₂, -NHR, -SH etc.

All auxochromes have one or more non-bonding pairs of electrons. If an auxochromes is attached to a chromophore, it helps is extending the conjugation by sharing of non-bonding pair of electrons

Ex: When the auxochrome -NH₂ group is attached to benzene ring. Its absorption change from λ_{\max} 225 to λ_{\max} 280.

ABSORPTION AND INTENSITY SHIFTS IN THE UV SPECTROSCOPY

Absorption and intensity shifts are four types:

a) Bathochromic effect (Red shift):

Bathochromic shift is an effect by virtue of which the **absorption maximum is shifted towards the longer wavelength** due to the presence of an auxochrome (or) change in solvents.

The $n-\pi^*$ transition of carbonyl compounds observes bathochromic (or) red shift.

Ex: The $n \rightarrow \pi^*$ transition for carbonyl compound gives bathochromic shift (increasing of wavelength) when the polarity of solvent is decrease, the negatively charge present on oxygen atom delocalized more due to red shift.

b) Hypsochromic shift (Blue shift):

This type of shift is an effect by virtue of which **absorption maximum is shifted towards the shorter wavelength**.

Generally it is caused due to the removal of conjugation (or) by changing the polarity of the solvents.

Ex: Aniline shows blue shift (decreasing of wavelength) in acidic medium and an unshared pair on nitrogen of aniline is not available for delocalization in cation, so that wavelength will be decrease.

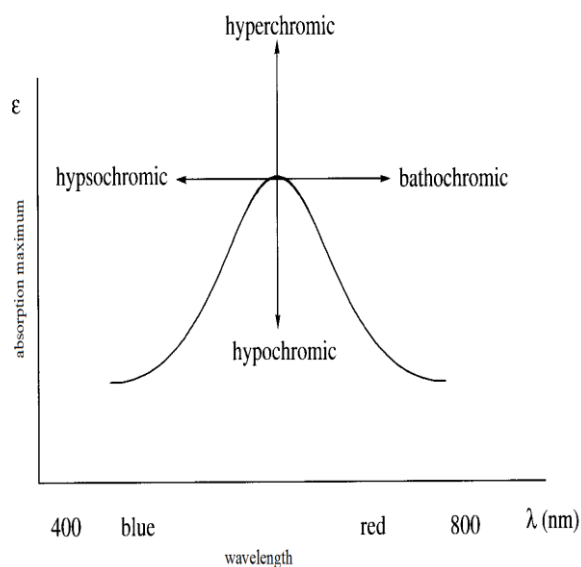
c) Hyperchromic effect: Hyperchromic shift is an effect by virtue of which **absorption maximum increases**.

The introduction of an auxochrome in the compound generally results in the hyperchromic effect.

d) Hypochromic effect:

Hypochromic effect is defined as the effect by virtue of **absorption maximum decreases**.

Hypochromic effect occurs due to the distortion of the geometry of the molecule with an introduction of new group.



APPLICATIONS OF UV SPECTROSCOPY**1. Detection of functional groups:**

UV spectroscopy is used to detect the presence or absence of chromophore in the compound. This technique is not useful for the detection of chromophore in complex compounds. The absence of a band at a particular band can be seen as an evidence for the absence of a particular group.

Ex: If the spectrum of a compound comes out to be transparent above 200 nm than it confirms the absence of _____.

a) Conjugation b) A carbonyl group c) Benzene or aromatic compound **d) Bromo or iodo atoms.**

2. Detection of extent of conjugation:

The extent of conjugation in the polyenes can be detected with the help of UV spectroscopy. With the increase in double bonds the absorption shifts towards the longer wavelength. If the double bond is increased by 8 in the polyenes then that polyene appears visible to the human eye as the absorption comes in the visible region.

3. Identification of an unknown compound:

An unknown compound can be identified with the help of UV spectroscopy. The spectrum of unknown compound is compared with the spectrum of a reference compound and if both the spectrums coincide then it confirms the identification of the unknown substance.

4. Determination of configurations of geometrical isomers:

It is observed that **cis-alkenes** absorb at different wavelength than the **trans-alkenes**.

- The two isomers can be distinguished with each other when one of the isomers has non-coplanar structure due to steric hindrances.
- The cis-isomer suffers distortion and absorbs at lower wavelength as compared to trans-isomer.

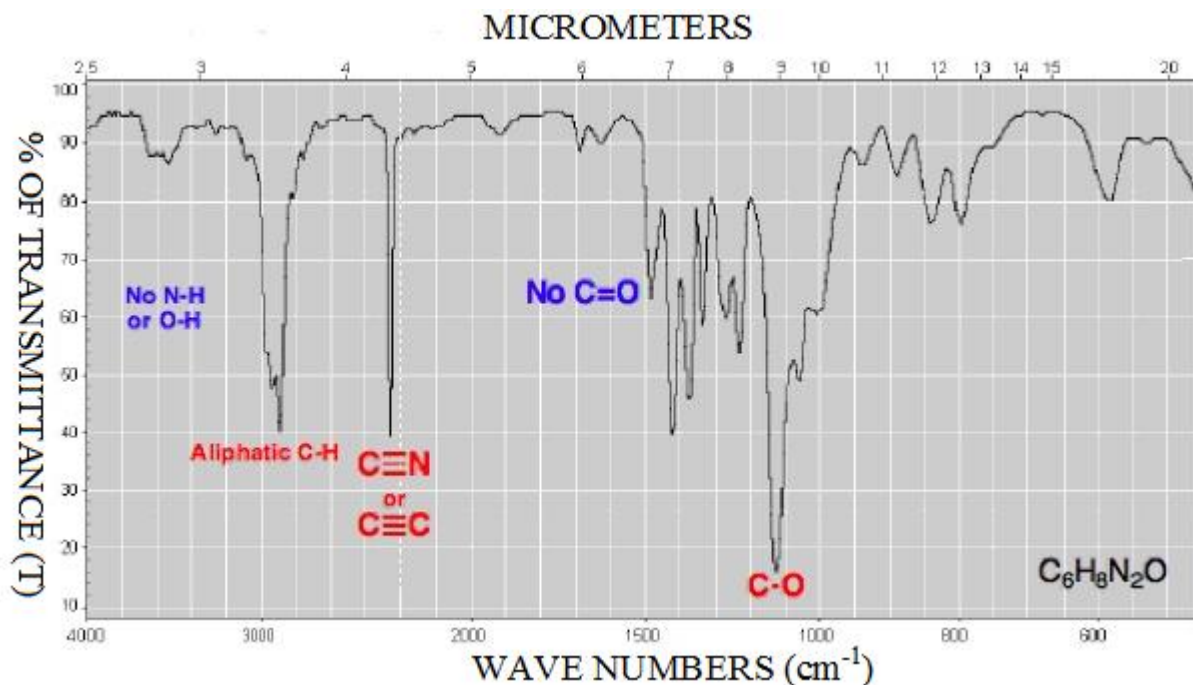
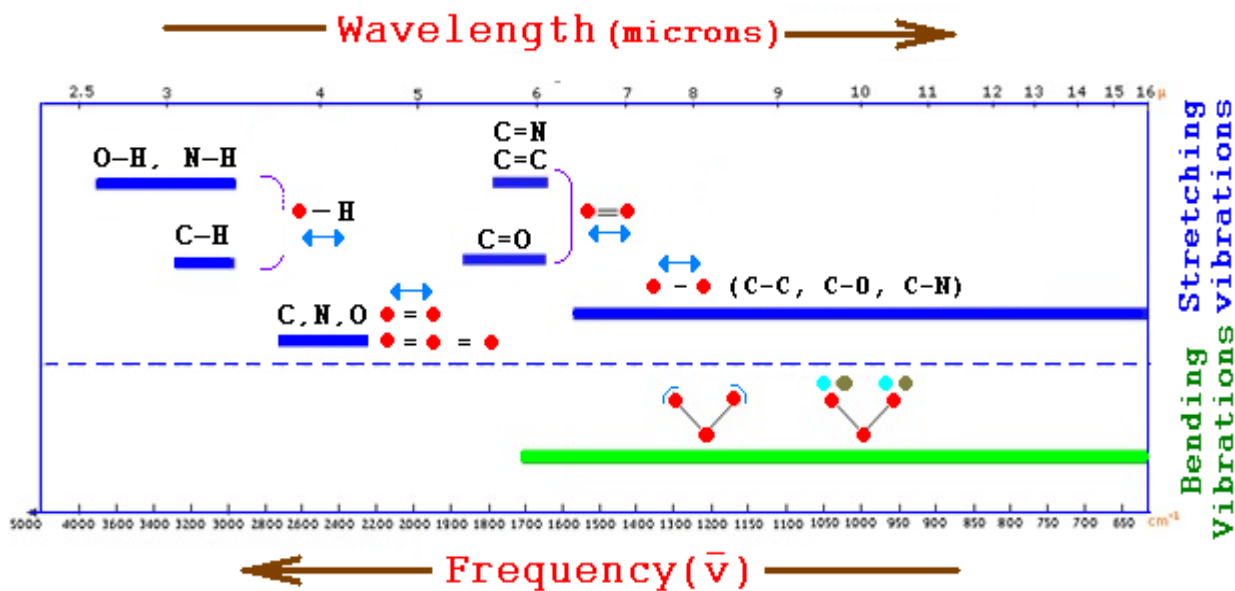
5. Determination of the purity of a substance:

Purity of a substance can also be determined with the help of UV spectroscopy. The absorption of the sample solution is compared with the absorption of the reference solution. The intensity of the absorption can be used for the relative calculation of the purity of the sample substance.

INTRODUCTION TO IR SPECTROSCOPY

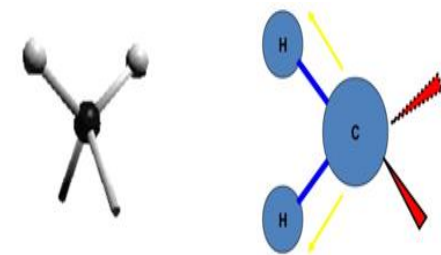
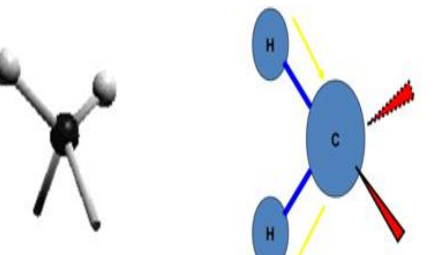

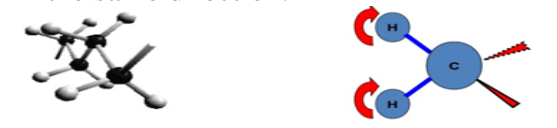
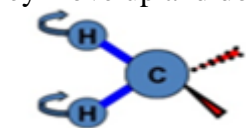
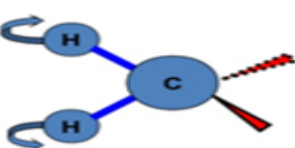
IR spectroscopy chart consist different regions of various kinds of vibrational bands. Absorption bands in the region are usually because of stretching vibrations of diatomic units.

1. Group frequency region is the region from 4000 to 1450 cm^{-1} .
2. Fingerprint region is the region from 1450 to 600 cm^{-1} .



STRETCHING AND BENDING VIBRATIONS

IR radiation does not have enough energy to induce electronic transitions as seen with UV. Absorption of IR is restricted to compounds with small energy differences in the possible **vibration and rotational states**. Vibrations are two types as follows:

Stretching-Vibrations	Bending Vibrations.
<ul style="list-style-type: none"> Stretching Vibrations are formed due to the vibration along the line of bond. Bond length will be change due to stretching vibrations. It occurs at higher energy ($4000-1250\text{cm}^{-1}$). These are two types: <ol style="list-style-type: none"> Symmetrical stretching. Asymmetrical stretching. 	<ul style="list-style-type: none"> Bending Vibrations are formed due to the vibration not along the line of bond. Bond length will not be change due to bending vibrations. It occurs at lower energy ($1400-666\text{cm}^{-1}$). These are two types: <ol style="list-style-type: none"> In plane bending (scissoring and rocking) out plane bending (wagging and twisting).
<ul style="list-style-type: none"> In symmetrical stretching two bonds length increase (or) decrease in simultaneously. <div style="text-align: center;">  </div> <ul style="list-style-type: none"> In asymmetrical stretching, one bond length increases and other bond length decreases. <div style="text-align: center;">  </div>	<ul style="list-style-type: none"> In scissoring the bond angles are decreases. <div style="text-align: center;">  </div> <ul style="list-style-type: none"> In rocking the movement of atoms takes place in the same direction. <div style="text-align: center;">  </div> <ul style="list-style-type: none"> In wagging two atoms move to one side of the plane and they move up and down the plane. <div style="text-align: center;">  </div> <ul style="list-style-type: none"> In twisting one atom moves above the plane and another atom moves below. <div style="text-align: center;">  </div>

PRINCIPLE OF IR SPECTROSCOPY

Infra-red spectroscopy is an important spectroscopy which gives almost complete information about the **structure of a compound**. The infra-red spectrum is containing a large number of absorption bands which provides much information about the molecule's structure.

The absorption of infrared radiations can be expressed either in terms of **wavelength** or **wave number**.

$$\text{Wave length (cm)} = 1 / \text{wave number (cm}^{-1}\text{)}$$

The intensity of bands observed in IR spectrum is expressed in terms of **transmittance** (T) or **absorbance** (A).

$$A = \log_{10} (1/T)$$

Because of absorption of infra-red radiation, molecules become excited and move to lower to higher vibrational level. Each vibrational level is associated with a number of spaced rotational levels. Hence the absorption of infra-red caused to effect vibrational as well as rotational level and also called as vibrational- rotational spectra.

Region	Wavelength range (nm)	Wave number range (cm ⁻¹)
Near	0.78 - 2.5	12800 – 4000
Middle	2.5 – 50	4000 – 200
Far	50 - 1000	200 - 10

INSTRUMENTATION AND WORKING OF IR SPECTROSCOPY

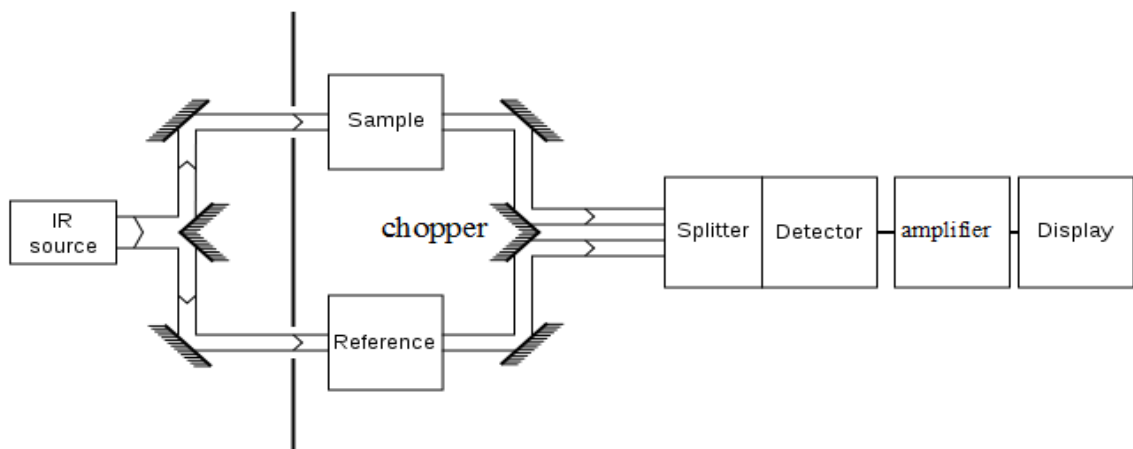
There are mainly two components in IR spectroscopy instrument, Source and detectors.

Source of IR spectrometer is **Nernst glower** (mixture of the oxides of Zr, Y and Er) and another source is **Globar(SiC)**

- The rod is electrically heated upto **1773° K** temperature to produce Infrared radiations; to change these IR radiations to monochromatic light, optical prism (or) grating can be used.
- Sodium chloride (or) other alkali metal halides is the best material to form prism.
- Cell container as they are transparent in Infra-red region. Light beam is split into two beams; one is **sample beam** and another beam is the **reference beam**. Due to absorption of radiation

by sample compound, the intensity of sample beam decreases. Hence there will be some difference in intensity of reference beam and sample beam.

- These two beams allow to fall on the **segmented mirror (chopper)** with the help of two supporting mirror. The segmented mirror also known as **chopper** rotates at a definite speed reflects the sample and reference beams to a monochromatic grating.
- As the grating rotates, it sends individual frequencies to the detector **thermopile** which convert IR energy to electrical energy.
- This is than amplified by using **amplifier**. Because of the difference in intensity of both beams, alternating current starts flowing from the detector to amplifier.



- The amplifier is coupled with a small motor which drive an optical wedge and further coupled with a pen recorder used to draw absorption bands on the calibration chart.

SELECTION RULES OF IR SPECTROSCOPY

The absorption of infrared radiations is possible by only those bonds of molecule which can show a change in **dipole moment** by the absorption of radiations. Such types of vibrational transitions which involve the change in dipole moment are known as **infra-red transitions**. However those vibrational transitions which are not accompanied by the change in dipole moment are not directly observed and called as infra-red inactive transition.

Ex: the vibrational transitions of C=O , O-H , N-H etc. bands are accompanied by the change in dipole moment, hence absorbed strongly in IR region.

While some other transitions like C-C bond in symmetrical alkene and alkyne are IR inactive transitions. Hence some of the fundamental vibrations are infra-red active and some are not. It governed by the selection rule.

1. If a molecule has a center of symmetry, then the vibrations are Centro symmetric and are inactive in the infra-red region but active in Raman, known as active vibrations.
2. The vibrations which are not Centro symmetric are active in infra-red region but inactive in Raman, called as forbidden vibrations.
3. Since the absorption of infra-red region is quantized, a molecule of the organic compound will show a number of peaks in the infrared region.

There are two important selection principles:

1. Only those transitions are permitted in which the vibrational quantum number (ν) changes by ± 1 . The transitions correspond this change are known as fundamental vibration tones. However vibrations of ± 2 , ± 3 , etc. equivalent to harmonic tones are known as forbidden transitions, which are not permitted.
2. The absorption of radiation can be possible only when the dipole moment of the whole molecule changes due to certain molecular vibrations.

IR SPECTROSCOPY CHART

IR spectroscopy chart consist different regions of various kinds of vibrational bands. The region from 1450 to 600 cm^{-1} is called as fingerprint region and the absorption bands in the 4000 to 1450 cm^{-1} region are usually because of stretching vibrations of diatomic units, and known as the group frequency region.

IR Absorptions of Common Functional Groups	
<i>Functional Group</i>	<i>Absorption Location (cm^{-1})</i>
Alkane (C-H)	2,850–2,975
Alcohol (O-H)	3,400–3,700
Alkene (C=C) (C=C-H)	1,640–1,680 3,020–3,100
Alkyne (C=C) (C=C-H)	2,100–2,250 3,300
Nitrile (C=N)	2,200–2,250
Aromatics	1,650–2,000
Amines (N-H)	3,300–3,350

APPLICATIONS OF IR SPECTROSCOPY

This technique is quite useful to predict the presence of certain functional groups which absorb at definite frequencies. It is widely used in different industries like organic synthesis, agriculture soil analysis and biochemical industries for the analysis of complex biological molecules like proteins, nucleic acid and lipids.

The main benefit of this technique is that some of the applications of IR spectroscopy are as follows.

1. Identification of functional group and structure elucidation:

- The identity of an organic compound is confirmed if its finger print region ($1400-1900\text{ cm}^{-1}$) exactly matches with the known spectrum of that compound.
- As compounds containing the same functional group may have similar absorptions above 1500 cm^{-1} but they differ considerably in the finger print region.

2. Identification of structure of substances:

- Infra red spectroscopy is used to establish the structure of an unknown compound.
- All functional groups present in a molecule absorb at their characteristic wave number and the shift due to environment effect can be easily observed in the spectrum.
- From the data available, the whole structure of a molecule can be predicted.
- IR spectrum cannot identify the presence of enantiomers as they show similar IR spectra.

3. Study of the progress of a chemical reaction:

- Infra red spectroscopy is quite useful for studying the rate and progress of a chemical reaction.
- For example, the reduction of a ketone to a secondary alcohol can be detected easily. As the absorption band of a ketone is observed at about 1710 cm^{-1} .
- With the progress of the reaction, the band of $>\text{C}=\text{O}$ group diminishes and the band of $-\text{OH}$ group at 3300 cm^{-1} appears.

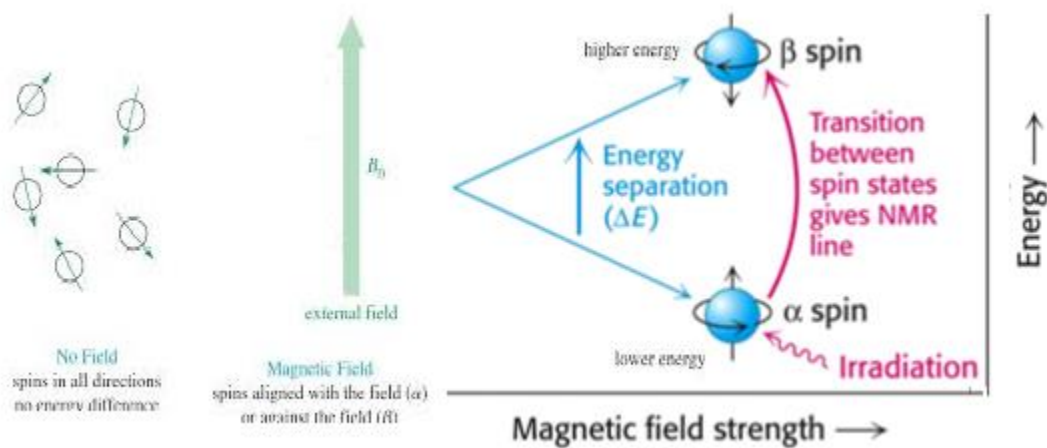
4. Detection of impurities Infra-red:

- Infra red spectroscopy is also useful in the detection of impurity in a compound by comparing its spectrum with the spectrum of the authentic sample of the compound. A pure sample always consists of sharp peaks and bands while the impure sample will have poor bands with some additional bands.

5. **Quantitative analysis:** The quantitative analysis of an organic mixture can be done by measuring the intensities of the absorption bands of each component.

PRINCIPLE OF NMR SPECTROSCOPY

- The principle behind NMR is that many **nuclei have spin** and **all nuclei are electrically charged**.
- If an external magnetic field is applied, an energy transfer is possible between the base energy to a higher energy level (generally a single energy gap).
- The energy transfer takes place at a wavelength that corresponds to radio frequencies and when the spin returns to its base level, energy is emitted at the same frequency.
- The signal that matches this transfer is measured in many ways and processed in order to yield an NMR spectrum for the nucleus concerned.
- The principle of nuclear magnetic resonance is based on the **spins of atomic nuclei**.
- The magnetic measurements depend upon the spin of unpaired electron whereas nuclear magnetic resonance measures magnetic effect caused by the spin of protons and neutrons.
- Both these nucleons have intrinsic angular momenta (or) spins and hence act as elementary magnet.



- The existence of nuclear magnetism was revealed in the hyper fine structure of spectral lines.
- If the nucleus with a certain magnetic moment is placed in the magnetic field, we can observe the phenomenon of space quantization and for each allowed direction there will be a slightly different energy level.
- NMR active: ^1H , ^{13}C , ^{15}N , ^{19}F , ^{31}P etc.

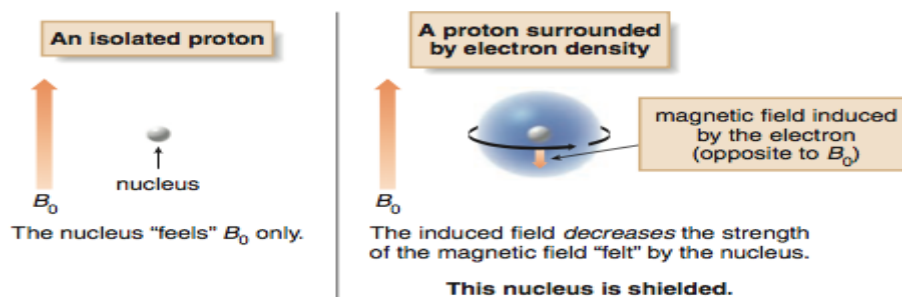
SHIELDING AND DESHIELDING OF NMR SPECTROSCOPY

The basic principle of NMR is to apply an **external magnetic field** called B_0 and measure the frequency at which the nucleus achieves **resonance**.

Electrons orbiting around the nucleus generate a **small magnetic field that opposes B_0** . In this case we say that **electrons are shielding the nucleus from B_0** .

Shielding:

- The **higher the electron density around the nucleus**, the higher the opposing magnetic fields to B_0 from the electrons, the **greater the shielding**.
- Because the **proton experiences lower external magnetic field**, it needs a **lower frequency to achieve resonance**, and therefore, the chemical shift shifts **upfield (lower ppm)** .

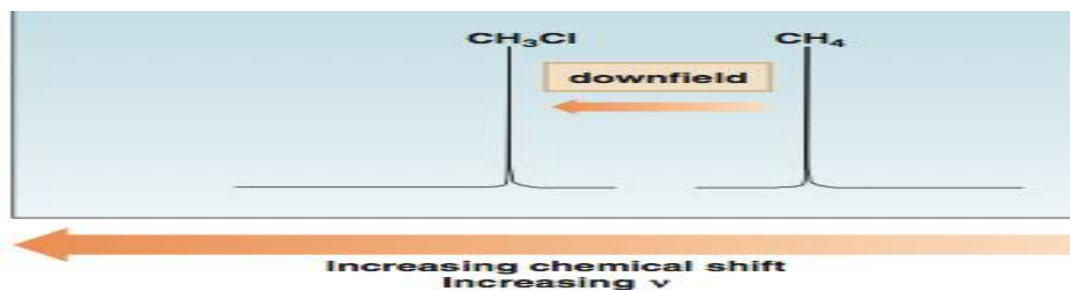


Deshielding:

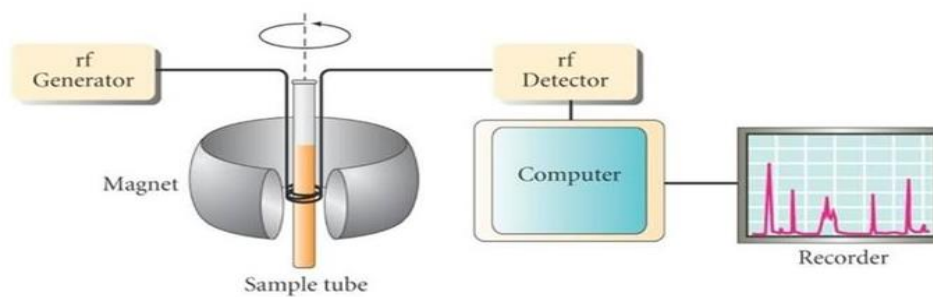
- If the **electron density around a nucleus decreases**, the opposing magnetic field becomes small and therefore, the nucleus feels more the external magnetic field B_0 , and therefore it is said to be **deshielded**.
- Because the **proton experiences higher external magnetic field**, it needs a **higher frequency to achieve resonance**, and therefore, the chemical shift shifts **downfield (higher ppm)**.

Example: Let us compare the chemical shift of CH_4 protons and CH_3Cl protons:

- Chlorine atom is an electronegative atom that will pull the electron density toward it (**electron withdrawing**), resulting in a **deshielding of the hydrogen nucleus**; an edit will fell higher external magnetic field B_0 increasing the resonance frequency and therefore, shifting to higher ppm.
- Hydrogen nucleus is shielded in the case of CH_4 and therefore, the peak appears on the lower ppm side.



INSTRUMENTATION OF NMR SPECTROSCOPY



The most important parts of an FTNMR instrument are:

- Magnet
- RF generator
- Sample chamber or probe
- pulse generator
- RF receiver
- Computer for data processing

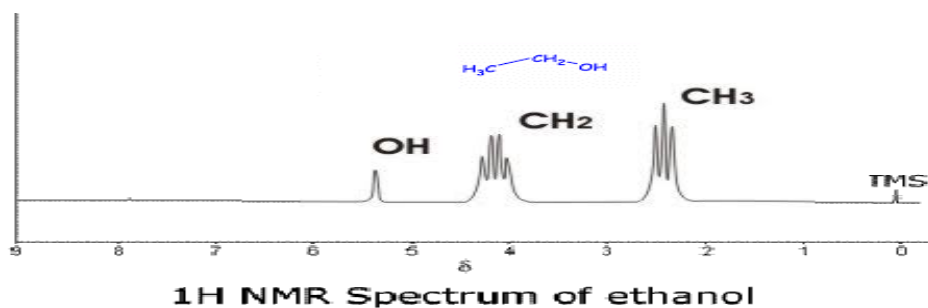
SELECTION RULE OF NMR SPECTROSCOPY

In NMR splitting of the signal based on the **$2nI+1$ rule**,

Where: I = spin of Hydrogen: H ($\frac{1}{2}$), n = neighboring group.

$$2n \left(\frac{1}{2}\right) + 1 = n + 1$$

Ex: NMR signal of ethyl alcohol (CH₃-CH₂-OH):



CH₃ (n+1rule where n=2hydrogens): 2+1=3(triplet)

CH₂ (n+1rule where n=3hydrogens): 3+1=4(quartet)

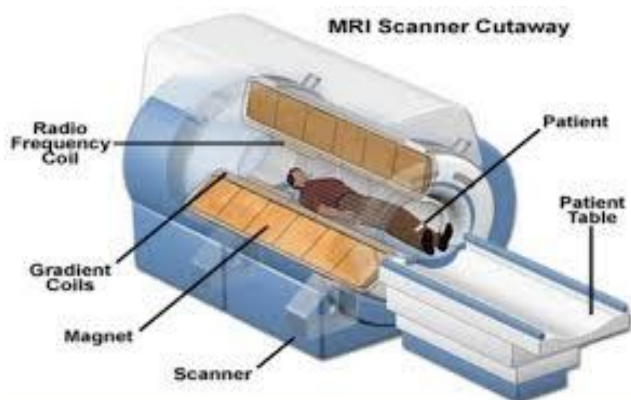
OH (n+1rule where n=0hydrogens): 0+1=1(singlet)

APPLICATIONS OF NMR SPECTROSCOPY

- It is useful to detect total number of protons present in the molecule.
- It is useful to distinguish between Cis and Trans isomers.
- It is useful in detecting aromaticity of molecule.
- It is also used to detect Hydrogen bonding in the molecule.
- In NMR spectra, different peaks give information about different atoms in a molecule according specific chemical environments and bonding between atoms. The most common isotopes used to detect NMR signals are ¹H and ¹³C but there are many others, such as ²H, ³He, ¹⁵N, ¹⁹F, etc., that are also in use.
- NMR has also proven to be very useful in other area such as environmental testing, petroleum industry, process control, earth's field NMR and magnetometers.
- Non-destructive testing saves a lot of money for expensive biological samples and can be used again if more trials need to be run. The petroleum industry uses NMR equipment to measure porosity of different rocks and permeability of different underground fluids.
- Magnetometers are used to measure the various magnetic fields that are relevant to one's study.

APPLICATIONS OF MAGNETIC RESONANCE IMAGING

The basic principle of MRI and NMR is the same. The mission of MRI makes use of the fact that the body tissue contains lot of water, the protons of which get aligned in a large magnetic field when a person is placed inside the powerful magnetic field of the machine; the protons align themselves with the direction magnetic field. This external magnetic field, applied on the nuclei, produce energy levels.



- Nuclear magnetic resonance imaging, better known as magnetic resonance imaging (MRI).
- It is an important medical diagnostic tool used to study the function and structure of the human body.
- It provides detailed images of any part of the body, especially soft tissue, in all possible planes and has been used in the areas of cardiovascular, neurological, musculoskeletal and iconological imaging.
- Unlike other alternatives, such as computed tomography (CT), it does not used ionized radiation and hence is very safe to administer.
- In many laboratories today, chemists use nuclear magnetic resonance to determine structures of important chemical and biological compounds.

MRI is used to diagnose (or) monitor the treatment conditions like the following diseases:

- Brain Tumors
- Trauma
- Infectious Diseases
- Pediatric Metabolic Disorders
- Alzheimer's disease

Learning objectives:

After completion of this unit the student should be able to:

- Principles of spectroscopy.
- Selection rules and applications of electronic spectroscopy.
- Selection rules and applications of vibrational spectroscopy.
- Selection rules and applications of rotational spectroscopy.
- Selection rules and applications NMR Spectroscopy.
- Nuclear magnetic resonance Spectroscopy - chemical shift.
- Introduction and Applications of Magnetic resonance imaging.

Short Answer Questions:

1. Define the term Auxochrome with example.
2. Explain the Selection rules of electronic spectroscopy.
3. Discuss the Selection rules of IR spectroscopy.
4. Write about Stretching and bending vibrations of molecules.
5. What are the applications of NMR spectroscopy?
6. Explain the Selection rules of NMR spectroscopy.
7. Define Chemical shift.
8. Explain Shielding and Deshielding effect of NMR spectroscopy.
9. Define the term Chromophore with example.
10. Explain different possible electronic transitions in UV-Spectroscopy of Carbonyl compound.

Descriptive Questions:

1. Describe the principle, instrument and applications of electronic spectroscopy (UV).
2. Describe the principle, instrument and applications of IR spectroscopy.
3. Describe the principle, instrument and applications of NMR spectroscopy.

4. Write about Electromagnetic spectrum (Wavelength and Frequency chart).
5. Write about the principle and applications of Magnetic Resonance Imaging (MRI).

Objective Questions:

1. According Laporte selection rule which of the following is forbidden transitions. **[d]**
 (a) g-u (b) u-g (c) Both (d) g-g

2. The range of group region- IR radiation is. **[b]**
 (a) 1446-666cm⁻¹ (b) 4000-1446cm⁻¹
 (c) 0-666cm⁻¹ (d) 4000 cm⁻¹-above

3. Which of the following is IR active molecule? **[b]**
 (a) H₂ (b) HCl (c) N₂ (d) O₂

4. The application of IR spectra from the following is... **[a]**
 (a) Functional group identification (b) un saturation
 (c) Hydrogen environment detection (d) none

5. In NMR spectroscopy the following waves are used **[a]**
 (a) Radio frequency waves (b) IR waves
 (c) UV waves (d) X-rays

6. The NMR value of TMS is the following. **[a]**
 (a) Zero δ ppm (b) one δ ppm
 (c) two δ ppm (d) three δ ppm

7. Spin selection rule singlet to singlet **[a]**
 (a) Laporte allowed (b) Laporte forbidden
 (c) Both (d) none

8. The number of NMR signals present in ethyl alcohol. **[c]**
 (a) One (b) Two
 (c) Three (d) Four

9. The distance between two NMR peaks is known as. **[c]**
 (a) Coupling constants (b) rotational constant
 (c) Chemical Shift (d) vibration constant

10. The full form of TMS **[a]**
 (a) Tetra methyl silane (b) Tri methyl silane
 (c) Tetra methoxy silane (d) Tetra Meta silane

Fill in the blanks:

1. Another name of the Ultra violet spectroscopy is **Electronic spectroscopy**.
2. According laprote selection rule **g-u** and **u-g** are the allowed transitions.
3. **Tungsten lamp (or) H₂-lamp (or) D₂-lamp** is the source of UV spectroscopy.
4. **200 -400 nm** is the wavelength range of the UV spectroscopy.
5. **1446-600 Cm⁻¹** is the finger print region in the IR spectroscopy.
6. **Nernest filament (or) Globber(or) hot quartz** is the source of IR spectroscopy.
7. **Nuclear Magnetic Resonance** is the full form of NMR spectroscopy.
8. **60 and 800 MHz** is the radio frequency (RF) range in NMR spectroscopy.
9. Chemical shift in NMR spectroscopy is expressed with **δ** symbol.
10. **TMS(tetra methyl silane)** is used in NMR as reference solvent.