frepency of Intra molecular hydrogen Bonding do not get change and occurs at higher Frepency than Intermolecular Hydrogen Bonding Molecules.

5. Kinetics of a Reaction :- The progress of a reaction can be analyzed by IR Spectroscopy

Nuclear Magnetic Resonance Spectroscopy

NMR is the Study of transitions of a nucleous from one Spin State to another on the absorption of Radio frepency waves when placed under magnetic field

Principle of NMR Spectroscopy

Nuclear spin Quantum Number :- (I)

Nucleous = Protons + Neutrons

Spin of Proton and Neutron $\pm \frac{1}{2}$

Range of Radiofrequency = 4 - 900 MHz

If spin of Both is clockwise [$(+\frac{1}{2})$ spin]

If spin of Both is Antibonding then Spin is $(-\frac{1}{2})$

(H) → $+\frac{1}{2}$ (β-orientation)
→ $-\frac{1}{2}$ (α orientation with magnetic field)

for Exp $^{2}_{1}D$ 1 = Proton
1 = Neutron

→ If Spin of Proton and Neutron is parallel then $I = \frac{1}{2} + \frac{1}{2} = 1$

→ If spin of Proton and Neutron is Antiparallel $I = \frac{1}{2} - \frac{1}{2} = 0$

(I) Spin Quantum Number is the fixed property of a nucleus
It Can be found Using the Rules

(1) If atomic number and mass number are even
$I = 0$
Exp $^{4}_{2}He$, $^{12}_{6}C$

(2) If atomic number is odd and mass number is even $I = 1, 2, 3, \ldots$

^{13}C, ^{1}H, ^{19}F, ^{14}N, ^{17}O, ^{31}P gives NMR

Exp $^{14}_{7}N$, $^{10}_{5}B$

③ When atomic number is odd & even and mass number is odd then $I = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$...

exp $_{1}H^{1}$, $_{9}F^{19}$, $_{11}^{23}Na$

NMR Active Molecules – when $I \neq 0$

Inactive – when $I = 0$

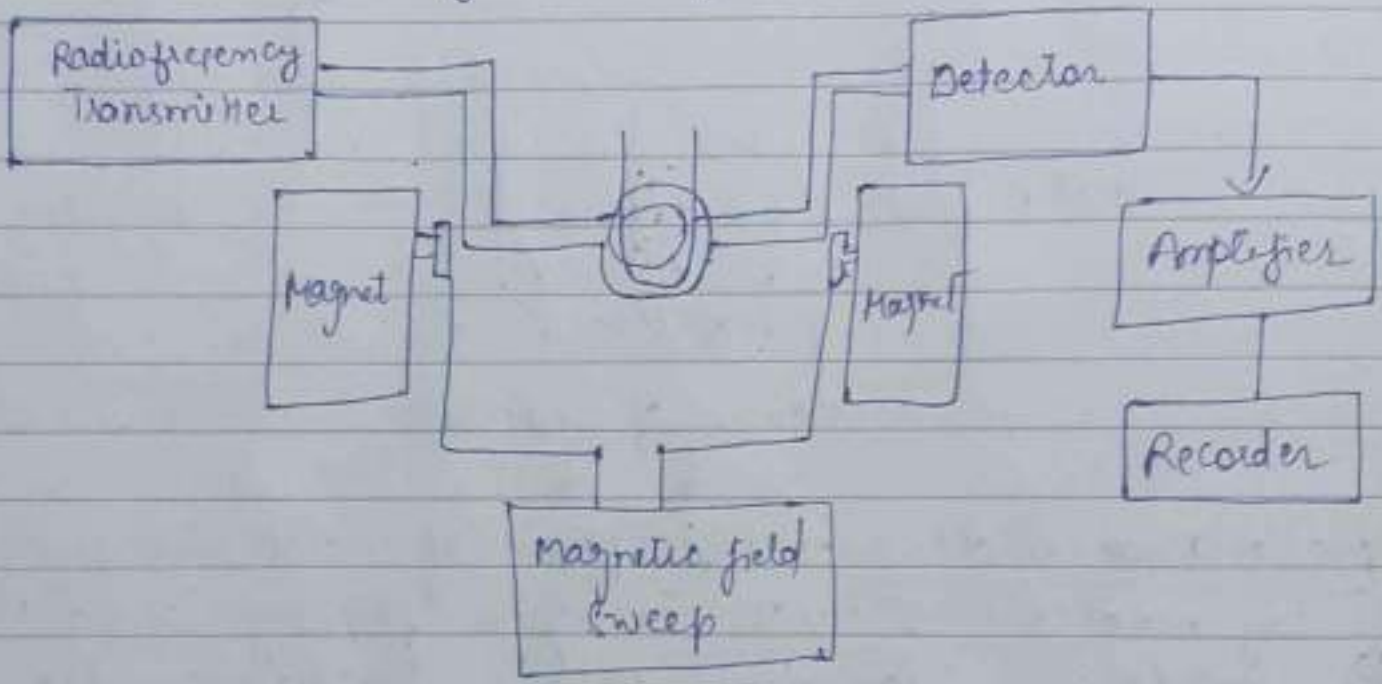
Instrumentation of NMR

Instrument used is NMR spectrometer

Components are

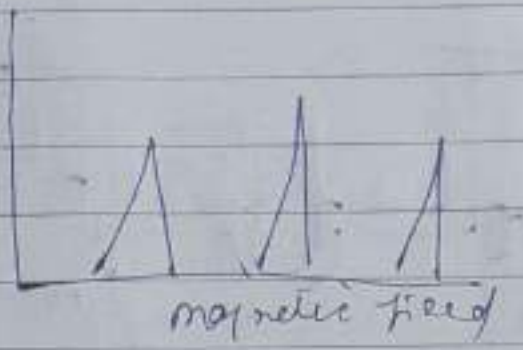
1) Radio frequency Transmitter
2) Sample Holder
3) Magnets and magnetic field Sweep
4) Detector
5) Amplifier
6) Recorder

Block Diagram of NMR Spectrometer



Sample is kept in to sample holder which is kept under the influence of magnets whose magnetic field is controlled from magnetic field sweep. Radio waves are absorbed by the sample and signals are converted in to electrons by the detector and then clearification is done by Amplifier which then sent to Recorder to Record NMR Spectra

The absorption Energy $y(v) = \frac{g \mu_N B}{h}$



Signals of NMR

Relaxation Process → Absorption of Radio frequency by nucleous results in spin flipping and undergoes Transition which increases the population of nuclei in the excited state. A state shows where no of nuclei is equal in both states which represents nuclei is Relaxing and no absorption occurs. But in actual case the nuclei in the excited state lose energy and return to ground state by different processes called Relaxation process which are of two types.

1) Spin - Spin Relaxation → When transfer of (from the Excited State) energy occurs to the neighbouring nuclei Spin-Spin Relaxation occurs. It do not produce any change in the population of nuclei from ground to Excited State.

2) Spin - Lattice Relaxation :- It is the transfer of energy by a nucleous form the Upper State to Surrounding in the form of Translational, Rotational and Vibrational energy.

Proton Magnetic Resonance Spectroscopy :-
or ^1H NMR Spectroscopy

It refers to the NMR of nucleus of Hydrogen Nucleous of Hydrogen Contains only one Proton It is mostly useful in the study of structure of unknown Compounds. It is also known as Proton NMR Spectroscopy.

Proton = Hydrogen

Information obtained from NMR

1) Number of Signals → No. of signals indicates the no of protons present in the compound. There are two kinds of proton present in a molecule.
   1) Equivalent proton → which is having same env. or lie in same plane.
   2) Non Equivalent proton → which is having different env. or lie in different plane

Exp

Equivalent Proton — CH_4 (a) — all four hydrogen lie in same plane and env.

Non Equivalent Proton — CH_3CH_2 (b, a) — 2 different protons means 2 signals.

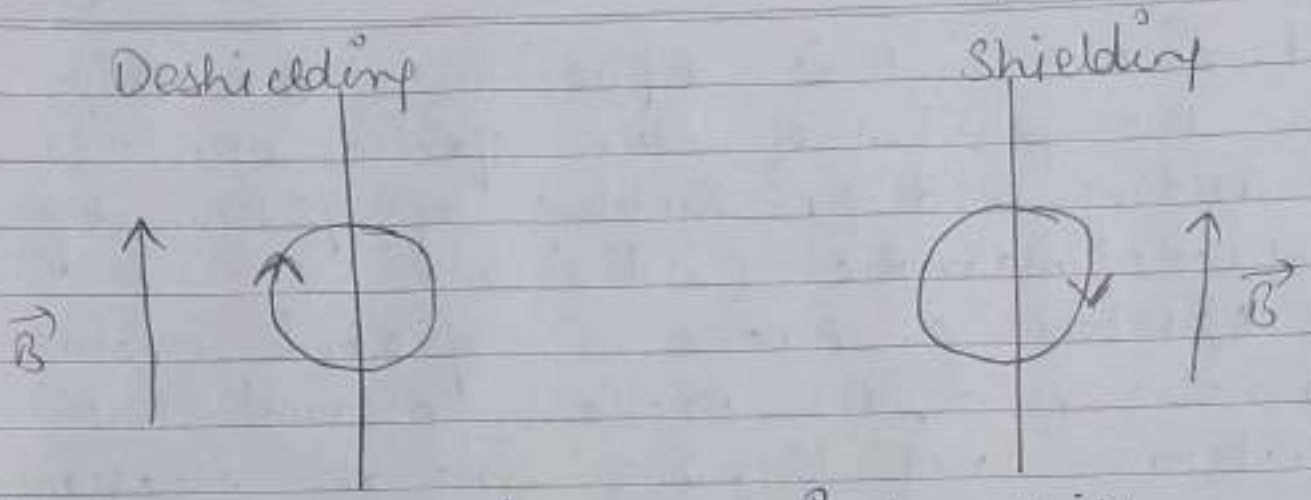
2.) Position of Signals :- Equivalent proton gives NMR signal at same position and Non equivalent proton give NMR signal at different positions. Posihon of a signal is determined on the Basis of Chemical Shift

"Chemical shift is defined as the shift in the position of NMR spectra due to shielding and Deshielding of protons by "induced magnetic field"

→ When a nucleous is placed under magnetic field, the electrons around the nucleous start behaving like an electron Bar magnet and produces an induced ($\vec{H}$) magnetic field. The direction of Induced magnetic field either oppose or Reinforces the Applied Magnetic field ($\vec{B}$). Thus Possibilities are there

→ If the direction of Induced magnetic field is opposite to the direction of Applied magnetic field than the field felt by the proton get decreased it is called "Shielding"

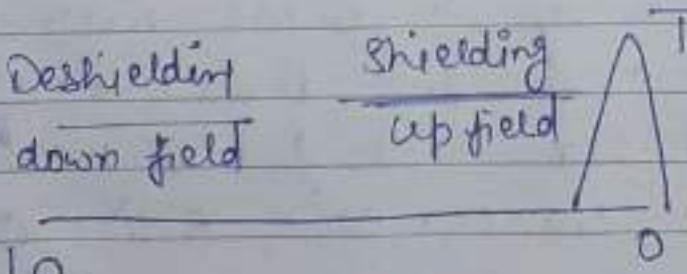
→ If the direction of Induced magnetic field is along the direction of ($\vec{B}$) than field felt by proton increases it is called Deshielding



Position of Signal = chemical shift

→ But to know where shielding and Deshielding occurs we must have an Reference Compound

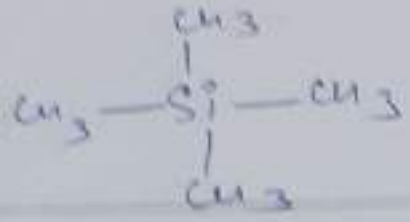
TMS is standard onto which there is shielding (Besides) and deshielding (far)



TMS = Tetramethyl Silane

Why it is used as Reference?

Ans There are some Reasons behind this

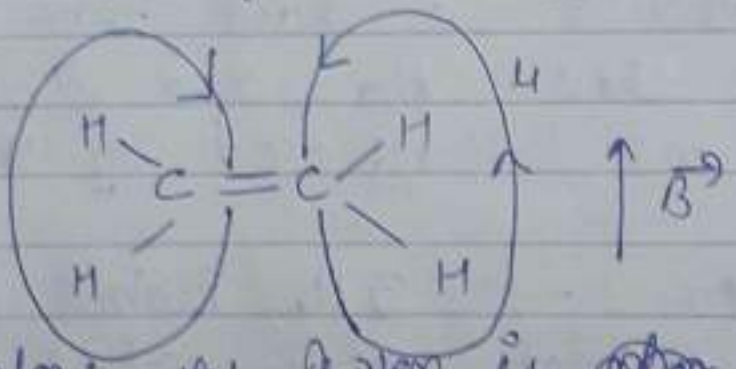


HITACHI
Inspire the Next

1.) All the 12 H are on the same plane so only one signal is there
2.) Due to low electronegativity of Silicon $\bar{e}$ density increased around (CH_3) group it results in shielding so it gives signal at upfield (Shielding) $\delta = 0$
3) It is chemically inert
4) Having low Boiling point so Removed easily after NMR

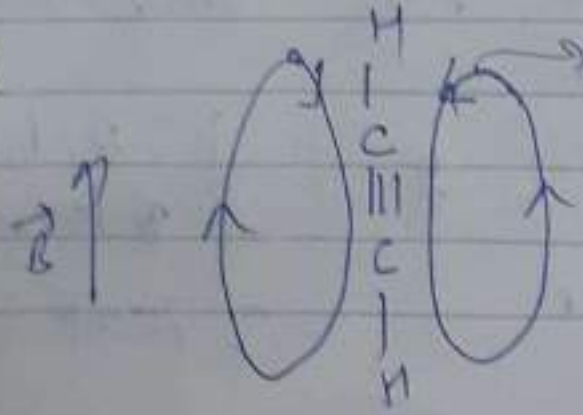
Chemical Shift of Some functional Groups

1) Alkene



Direction along the proton is Reinforcing the applied Magnetic field

2) Ethylene

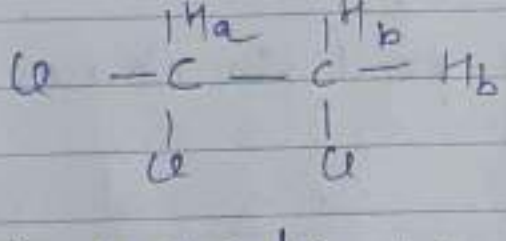


Direction along Proton opposed the direction of $\vec{B}$

Splitting of Signals

→ No of signals further splits in to no of peaks. Formula = $(n+1)$ peaks
where n = no. of Proton (adjacent)

For Example



Ha = $n = 2$
Ha = $(2+1)$ 3 Peaks
Hb = $(1+1)$ 2 Peaks
Hb $n = 1$

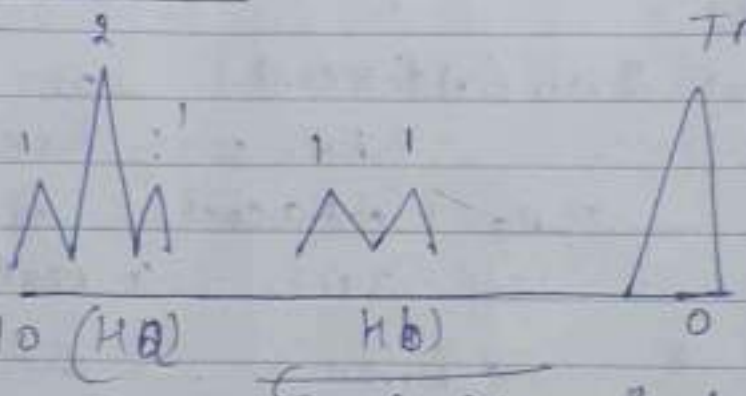
In this Molecule we have two kinds of proton are there Ha and Hb
Spin of one is affected by the other

For Ha Proton → 2 Hb Protons (adjacent)
→ The spin of Both Hb is along or against the applied Magnetic field.
So we have four combinations

$\vec{B}$ ↑↑ = 1
↑↓ or ↓↑ = 2 — 1 : 2 : 1 Intensity
↓↓ = 1 — 3 Peaks

For Hb Proton = 1 Ha Proton which is either along or opposite ; so two peaks are there (↑↓ or ↑↑) Intensity 1:1

Representation

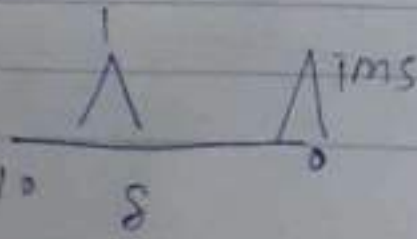


For Ha signal occurs at shielded Region due to two Cl groups (electronegativity)

Interpretation of Some Compounds

① $CH_3-\overset{O}{\overset{\|}{C}}-CH_3$ (Ha, Hb)

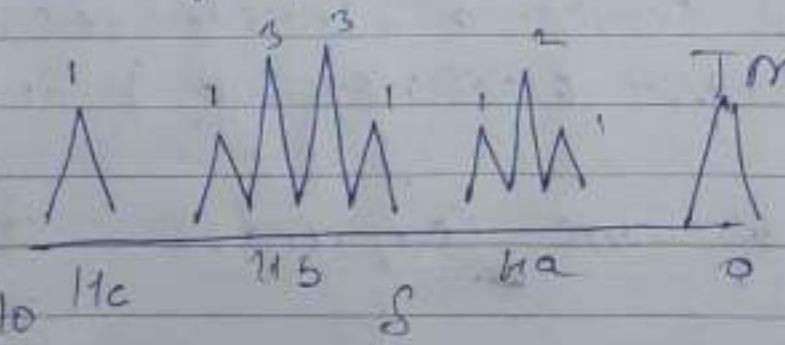
(a) only one kind of Proton
(b) only one Signal
(c) only one Peak



(2) $CH_3 - CH_2 - O - H$
Ha Hb Hc

(1) only three protons are there
(2) Three signals
(3) for Ha → 2 Hb (Adjacent) n = 2
(2+1) = 3 Peaks
for Hb — 3 Ha (Adjacent) n = 3
(3+1) = 4 Peaks
for Hc — no proton → one peak

(4) Position of signals



Surface characterisation Techniques

Surface Characterisation means the characteristics of a material associated with the properties of its surface

→ Measurements of surface area, surface Roughness, pore size Constitute surface characteristics.

→ Information on surface characteristics is very important for the applications of surfaces as semiconductors, heterogenous catalysts and also in biological Research.

Techniques Used in Surface Characterisation

1. X-ray Photoelectron Spectroscopy
2. Auger Electron spectroscopy
3. Electron microscopy
   a) Scanning Electron Microscope
   b) Atomic Force microscope
   c) Transmission Electron microscope
   d) Probe or

Q- Differaction

→ It refers to various phenomena that in which there is slight bending of light as it passes around the edge of an object. The amount of the bending of light depends on the size of wavelength of light to the size of the object.

X-ray Differaction :- It is the most important technique used for the

Bending of Incident light = Size of wavelength / Size of Object

Identification of a crystalline material, their spacing and wavelength of the incident x-ray by using Bragg's law

When a beam of X ray is allowed to fall on a crystal surface at some angle (θ) called Incident angle and spacing b/w the crystal (d) act as a source of scattered Radiation

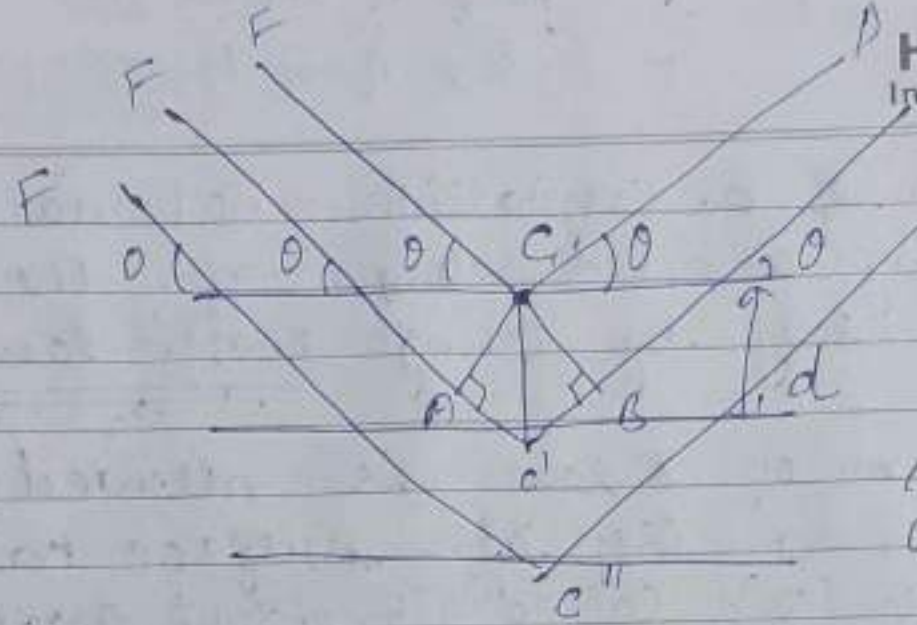
So when Beam strikes, a proton is scattered by the layer of atom at surface and again beam get scattered by the next atom having spacing d

Bragg developed a relationship between Xray and spacing

Path length FCD and FC'D'

FC'D' is longer than FCD by AC'B

$n\lambda = 2AC = 2d\sin\theta$



λ = wavelength
d = Spacing

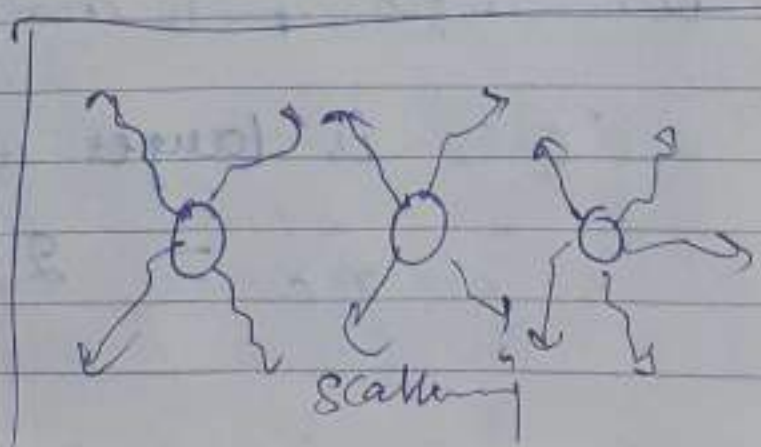
n = order of diffraction

Condition for diffraction

Diffracted beams are found to occur when reflections from plane of atoms interfere constructively.

There X-ray diffraction methods are

(1) Laue
(2) Rotating Crystal
(3) Powders



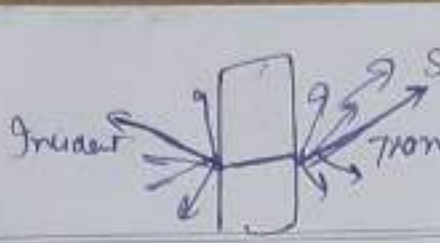
Scattering

→ It is a Physical process in which light get deviate from its path by one or more paths. Scattering may be due to collision between the molecules, atoms, electrons and other particles

→ Most of the spectroscopic technologies deals with the absorption of light. However Raman spectroscopy deals with scattering of light.

→ But it was Rayleigh who observed for the first time that On irradiation of a substance with monochromatic light, the scattered light is observed is in a direction perpendicular to the incident light. This is called Rayleigh scattering.

→ But Raman observed that along with Rayleigh scattering there are some frequencies which are different than incident light, these are known as Raman Lines.



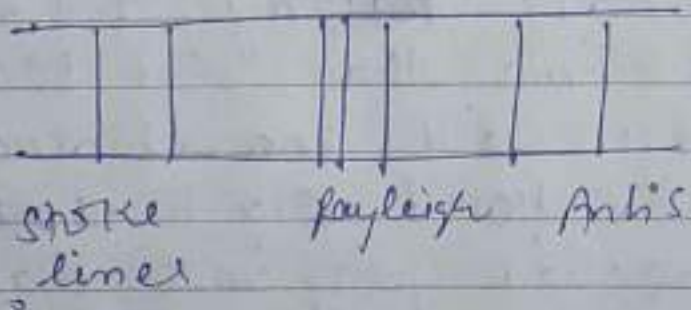
(1) Stoke lines → whose wavelength is greater than Incident light
(2) Anti stoke lines - less than Incident light

ν_i = frequency of Incident light
ν_s = " of scattered Radiation

$\Delta\nu = \nu_i - \nu_s$

$\nu_i > \nu_s$ → $\nu_s > \nu_i$

$\Delta\nu$ = +ve (Stoke lines) $\Delta\nu$ = -ve (Anti)



Applications

(1) Structure of Compounds
(2) Ionic equilibrium in solution
(3) ~~degree of hydrolysis of Light~~
study of Polymers.
(4)
(5) Both Organic and Inorganic samples are determined

Applications of X-ray Diffraction

→ Structure of Crystals
→ Characterisation of Polymers
→ Nature of Complexes
→ Organic Compounds can be Converted in to Crystalline derivatives

Magnetic Resonance Imaging (MRI)

→ It is a medical test that Physicians use to diagnose medical conditions.
→ It uses powerful magnetic field, Radio waves and a Computer to produce detailed pictures of the inside of your body.
→ It is used in variety of conditions within the chest, abdomen (Skin) to help to diagnose diseases like tumors of the chest, abdomen diseases of liver, such as cirrhosis heart problems and fetus in the womb of a pregnant woman.

HITACHI
Inspire the Next

Q How does the MRI equipment look like?

Ans is Traditional MRI is a large Cylinder - shaped tube surrounded by a circular magnet. We have to lie on a movable table that slides in to the centre of the magnet.

Q How does it works?

Ans It uses Radiofrepency pulses which re align the hydrogen atoms that naturally exists in our body without any chemical change in the tissue. As the hydrogen atoms return to their original alignment, they emits different amount of energy according to the type of body tissue from which they come. MRI Scanner Capture this energy and Creates a picture on the Computer.

Magnetic field is produce by pasing electric Current through wire coils in most MRI Patient do not come in Contact with electric field.

Application → Sodium ^{23}Na MRI used for analysis of blood

^{19}F for conc of F in various body parts

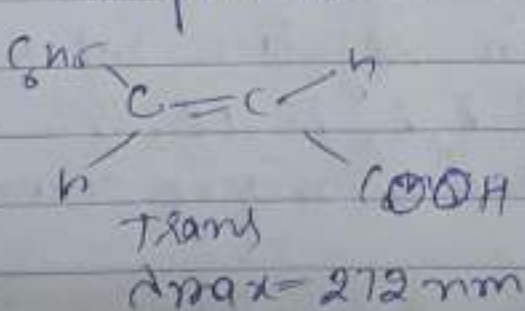
P, F, N, O → less abundant

MRI exams generally include multiple runs; some of which may last several minutes

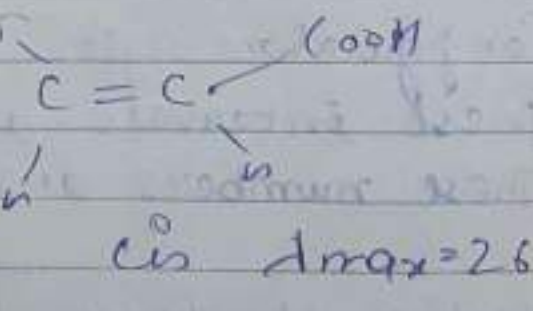
Entire process completes in 30-50 minute

Application Of UV visible

1. Identification of Functional Groups
2. Determination of Unknown Compound
3. Distinguish b/w Cis and Trans Compounds



Trans
$\lambda max = 272$ nm



Cis $\lambda max = 268$

4. Distinguish b/w Conjugated and non conjugated

$H_2C = CH - CH = CH_2$, $CH_2 = CH - CH_2 - CH_2 - CH_3$

5. Determination of Extention of conjugation
6. Quantitative analysis — unknown conc. can be find out.