PG. Semester – III
CC- X

PAGE:
DATE: / /

Proton Nuclear Magnetic Resonance. Spectroscopy- ^{1}HNMR

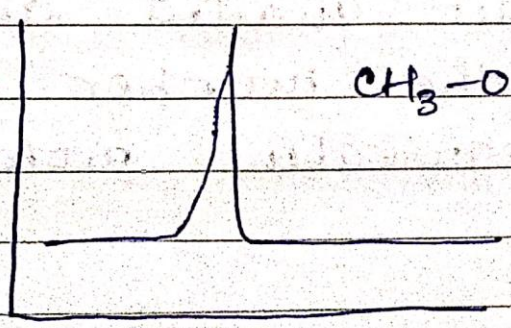
→ It is change in the spin state of a nuclear magnetic moment when the nucleus absorbs the electromagnetic radiation in strong magnetic field.

→ Two principal kind of informations are obtained from it

- The relation between different signals on a spectrum and different kinds of environments of hydrogen atoms in the molecules.

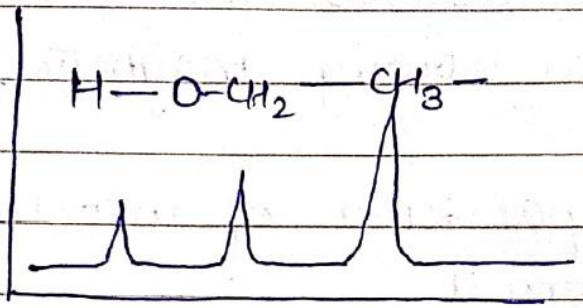
- The area under each signal is same ratio as the number of hydrogen atoms causing these signals.

eg: for Dimethyl ether



All the six hydrogen atoms are in the same environment and therefore show only one sharp signal.

now for ethyl alcohal



There are three type of H- atoms and therefore three peaks are observed. The ratio of peak area is 1:2:3.

In addition to these two, there is also the information about splitting the peak. The splitting patterns can be doublet, triplet, quartet and so on, depending on the number of neighbouring non-equivalent protons.

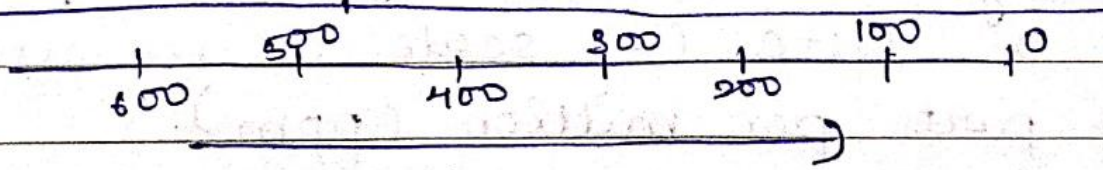
This splitting can be explained on the basis of n+1 rule, where n is the number of neighbouring protons.

This spin spin splitting helps to determine the molecular structure.

The spacing between the peaks is labelled as J, given the units of cycles per second or Hertz (Hz).

J is the coupling constant between two protons. It also gives information about molecular structure and stereochemical features.

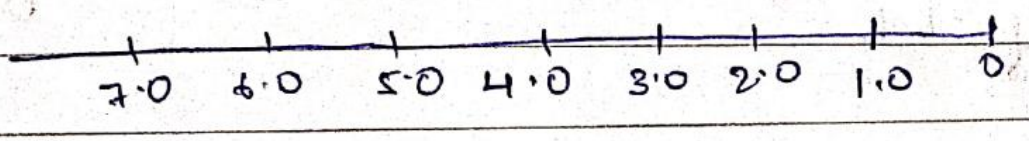
The PMR. Spectrum:- An Introduction:-



(a)

Shielded protons are upfield to the right (lower δ)

Deshielded



Chemical shift (δ)

The reference $\delta = 0$ is for Tetra methyl silane. The TMS is the internal standard for the sample.

The difference between chemical shift positions are measured between the reference (TMS) and the signals from the compound under examination.

The distance of value δ from TMS is is called chemical shift for the proton.

(b) The chemical shifts are measured along the bottom of the spectrum on a delta (δ) scale or in units of parts per million (ppm).

The chemical shift is proportional to strength of external magnetic field.

Chemical shifts are always small (< 5000 Hz)