Pg-3
Spectroscopy
R.N college

NMR – Nuclear Magnetic Resonance Spectroscopy

It involves the change in the spin state of a Nuclear magnetic moment when the nucleus absorbs Electromagnetic radiation in a strong magnetic field.

– There are two types of NMR Spectroscopy used

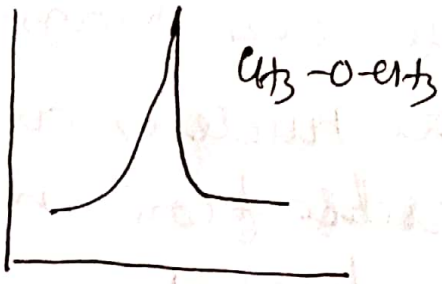
(I) H^1-NMR spectroscopy
(II) ^{13}C-NMR Spectroscopy

^1H-NMR Spectroscopy deals The Following kind of Informations

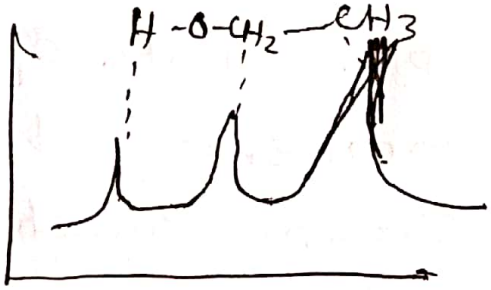
(I) The relation b/w the number of signals (or peaks) in spectrum and The different kinds of environments of the Hydrogen atoms in the molecule.

(IV) The areas underneath each signal are in the same ratio as the number of H atoms causing signals

Ex- CH_3-O-CH_3 has six H-atoms in identical average environments and one sharp resonance signals



Only one signal in dimethyl ether



Three signals in ethanol

However, in ethanol ~~dis~~ found in three different kinds of absorption peaks which shows three kinds of H-atom.

Hence ratio of three peaks are in 1:2:3 for OH, CH_2, CH_3 respectively.

(iii) The principal signal may get into smaller peaks i.e. spin-spin ~~coupling~~ splitting may be observed. The type of splitting (doublet, triplet, quartet etc) depends upon the no. of neighbouring non equivalent protons

ratio 0:4

(iv) The Spacing b/w the peaks as a results of spin-spin splitting is labelled as J (in the unit of cycle per second or Hz)

J = Coupling constant between two protons. The J values give further information on molecular structure and stereochemical features.

Ex- J value of between adjacent axial H in cyclohexane is 10-13 Hz while between axial & Equitorial or b/w two Equitorial H is 3-5 Hz

---

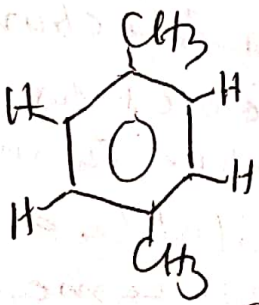
Prediction of Nmr Signals

(1) $CH_3-CH(OH)-CH_3$ 3 kinds of ^1H-nmr Signal

(2) $CH_2(-COOCH_2-CH_3)-CH_2(-COOCH_2-CH_3)$ 3 kinds " " "

(3) $CH_3-CH_2-CH_2-COOH$ 4 kinds " "

(4)



2 kinds :-
Area under the signals of CH_3 group (6H) is larger than that for benzene H in ratio 6 : 4 -

TMS – Tetramethyl Silane is most Suitable reference compounds

- TMS signal is used to define the zero position on the δ-scale
- The protons of TMS are known to come to resonance at exactly 60MHz. Thus zero Hz line is set at exactly 60MHz at the right hand side of spectral paper. When using 6MHz spectrometer
- Using 90MHz instrument, protons of TMS are known to come to resonance at exactly 90MHz. Hence zero Hz is set at exactly 90Hz
- TMS gives only peak at high field position for its protons relative to those in most Organic Compound
- The TMS signal occurs at the right edge of the spectrum and can be easily detected as Si is less electronegative than Carbon
- TMS is highly volatile and after NMR spectral measurement it can be easily removed.
- It gives intense sharp peak even at low conc.