FAQ's

Q.1. Define NMR spectroscopy.

Ans: NMR is the most powerful analytical tool currently available to an organic chemist. It allows characterization of a very small amount of sample (approximately 10mg), and is a non-destructive technique i.e., it does not destroy the sample. NMR spectra can provide vast information about a molecule's structure and can very often be the only way to prove what compound really exists. NMR can be used in conjunction with other types of spectroscopy and chemical analysis to fully confirm a complicated molecular structure.

Q.2. Describe in brief the principle of NMR.

Ans: Any nucleus that has either an odd atomic number or an odd mass number has a nuclear spin that can be observed by an NMR spectrometer. The proton is the simplest and also the most useful nuclear particle employed for organic characterization of samples in NMR analysis. NMR theory is reasonably complicated, involving the magnetic alignment of spins of different nuclei with respect to the alignment of the magnetic field that is externally applied.

Q.3. Give some important features of NMR spectroscopy.

Ans: Some important features of NMR spectroscopy are given below:

a) The number of different absorptions implies how many different types of hydrogen atoms are present.

b) The amount of shielding (chemical shift) is determined by the environment of each hydrogen atom, so we get information about the local electronic surroundings for each hydrogen atom.

c) The intensities of the signals tell us the number of identical hydrogen atoms.

d) The splitting of each signal tells us about the other groups proximate to the hydrogen atoms in question.

Q.4. What is meant by nuclear spin?

Ans: Nuclei have positive charges. Many nuclei behave as though they were spinning around their own axis. Anything that is charged and moves has a magnetic moment and produces a magnetic field. Therefore, a spinning nucleus acts as a tiny bar magnet oriented along the spin rotation axis. This tiny magnet is often called a nuclear spin.

Q.5. What are the different components of the NMR machine?

Ans: An NMR machine consists of:

a) A powerful, super-cooled magnet (stable, with sensitive control, producing a precise magnetic field).

b) A radio-frequency transmitter (emitting a very precise frequency).

c) A detector to measure the absorption of radiofrequency by the sample.

d) A recorder (to plot the output).

Q.6. What makes TMS a preferred standard for NMR interpretation?

Ans: The chemical formula of tetramethylsilane or TMS is $(CH_3)_4Si$. All of the protons on the methyl groups present in this compound are in the same electronic environment. Therefore, only one NMR signal will be generated in its NMR analysis. Furthermore, the compound consists of silicon whose electronegativity is less than that of the carbon atoms which prevents the deshielding effect in it. In addition to this, TMS is taken as a reference compound because of its inert quality that prevents it from reacting with the sample and its highly volatile nature that makes it easy to evaporate out of samples. Only a few compounds have a lower frequency reading

than TMS and it has 12 equivalent protons that read strongly on the NMR spectra.

Q.7. What is the significance of peak intensity in NMR?

Ans: Peak intensity is of great significance in NMR spectroscopy. The area of an NMR signal is known as the peak intensity, while as the height of an NMR signal is referred to as peak amplitude. Peak intensity is directly proportional to the number of nuclei contributing to the signal. Consequently, if the concentration of nuclei is known for a particular peak, it can be used as a standard.

Q. 8. List some disadvantages of NMR technique:

Ans. NMR has some disadvantages like

- Relatively large amount of sample is required to start with.
- Sample that is dissolved in solvent is preferred.
- It requires a long time scale.
- It is expensive.
- It is inherently not very sensitive technique for detecting impurities.

Q. 9. Which atoms are magnetically inactive?

Ans. The atoms that are magnetically inactive have even number of neutrons and even number of protons in their nucleus.

Q.10. Which atoms are magnetically active?

Ans. The atoms that are magnetically active have either of the following property:

- Odd number of neutrons plus protons (sum of the two) in their nucleus, as in case of ^{1}H and ^{15}N.
- Odd number of protons well as odd number of neutrons in their nucleus as in case of ^{2}H and ^{14}N.

Q.11. What are the different alignments that a magnetically active nucleus can adopt in presence of an external magnetic field?

Ans. When a magnetically active nucleus is placed in an externally applied magnetic field, it may exhibit two possible orientations. It may align its spin parallel or anti-parallel to the direction of applied magnetic field. In former case, the orientation is called low energy orientation while in later case, the orientation is called high energy orientation.

Q.12. Define the term precess.

Ans. Precess is a type of motion similar to gyroscope. It is a type of motion in which a body moves with an angle that varies cyclically. This type of motion is also called wobbling.

Q.13. Define population distribution.

Ans. In a given sample of a specific NMR active nucleus, nuclei are distributed throughout the various spin states with comparatively small energy barrier. Population distribution is the ratio of number of nuclei in the higher energy state to the number of nuclei in the lower energy state.

Q.14. Define Boltzmann distribution equation.

Ans. Boltzmann distribution equation is given below:

$$N_{upper} / N_{lower} = e^{-\gamma Bo/kT}$$

Here, 'N' values are the numbers of nuclei in the respective spin states, 'γ' is the magnetogyric ratio that relates the magnetic moment and the spin number for a specific nucleus (i.e., γ = precession rate/strength of the externally applied magnetic field), **h** is Planck's constant, $\mathbf{B_o}$ is the external magnetic field strength, **k** is the Boltzmann constant, and **T** is the temperature.

Q.15. What are continuous wave NMR spectrometers.

Ans. In continuous wave NMR spectrometers, the sample is held in a strong magnetic field, and the frequency of the source is slowly scanned

in a way similar in principle to optical-scan spectrometers. However, in some instruments, the source frequency is held constant while the magnetic field is scanned. These systems are currently obsolete except for a few wideline experiments that are performed in specialty solid-state NMR applications.