Hello students, today we're going to study NMR spectroscopic method. We're going to analyze & try to understand how NMR spectrum is taken for a compound and then using NMR spectroscopy you will understand how to find out the structure of a compound.

This is coming under Industrial chemistry subject with paper code ICD 101 and paper title Industrial chemical analysis. The title of the unit is Spectroscopy & Module name is basic principles in NMR spectroscopy.

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In this module you will come across some important words like NMR active and non-active nuclei, degenerate energy levels, effective magnetic field strength, electronic environment around the protons, signal splitting etc.

Using these terminologies you can understand and try to find out what are NMR active and non-active nuclei? How NMR spectrum is obtained? Why signal splitting takes place in certain cases? Meaning of electronic environment around the protons, difference between <u>effective</u> magnetic field felt by proton and applied magnetic field? Etc.

Basically nuclei with nuclear spin quantum number I > 0 are NMR active. Nuclei with odd number of protons and or neutrons are NMR active. E. g.  $_{1}H^{1}$ ,  $_{6}C^{13}$ ,  $_{7}N^{14}$ ,  $_{9}F^{19}$ ,  $_{15}P^{31}$ . However, if we consider  $_{6}C^{12}$ ,  $_{8}O16$ ,  $_{16}S^{32}$  are NMR inactive nuclei.

When the nucleus spins, it generates a small magnetic field which is randomly oriented in space in absence of external magnetic field. The number of orientation for a nuclei having spin quantum number or angular momentum I is given by equation 2I+1. If we take example of hydrogen having spin quantum number I is equal to ½ will have two orientations possible. In presence of external magnetic field these nuclei either align themselves with the direction of the applied magnetic field or against it giving two different energy states. This can be explained in a simple diagram here. So you can see when the magnetic field is applied, how the nuclei are separated from each other? When the external magnetic field is removed, the energy states become degenerates. They acquire the original position with the same energy level.

To get NMR spectrum, compound can be placed in a magnetic field of constant strength & radiations of changing frequency can be passed through or vice a versa. In actual practice, it is convenient to keep frequency of radiation's constant & change the applied magnetic field. At some value of the applied magnetic field the energy required to flip the proton from  $E_1$  to  $E_2$ , that is from lower energy level to the higher energy level matches the energy of radiation, absorption occurs giving a signal. When the spin flips from  $E_1$  to  $E_2$ , which is from lower energy level to the higher energy level, the nucleus is said to be in resonance with the radiations absorbed and therefore the name for this particular spectroscopy is given as Nuclear Magnetic Resonance spectroscopy. Nucleus kept in the magnetic field is in resonance with the absorption of radiation.

The frequency at which the proton absorbs energy depends on the magnetic field felt by that proton, which is called as effective magnetic field strength. The effective field strength is not the same as that of applied magnetic field strength. The effective field strength felt by each proton depends upon the electron density at that proton and the presence of nearby protons. Therefore, at a given radiofrequency, all protons absorb at the same applied magnetic field but at a different effective magnetic field strength.

NMR spectrum is obtained by plotting applied magnetic field strength against the absorption which gives following information. A number of signals tell us how many different types of protons are present in the compound, positions of the signals indicate electronic environment around each proton, intensities of each signal indicate how many protons of each kind of present & splitting of signals into several peaks indicates the electronic environment of protons with respect to nearby protons.

These aspects can be explained very easily by considering the NMR spectrum of Ethyl bromide. If we look at the spectrum we see three different peaks, the extreme right peak is observed at 0  $\delta$  value is the reference peak. As we move from right to left we are coming to the first three peaks, which are denoted as A given by methyl group, CH<sub>3</sub>. If you look at the intensity there, the intensity of the peak is quite high, indicating this is given by three hydrogens. If we come to peak B, you can see the intensity is less than that of the peak A because it is given by two hydrogens. Even if you look at the pattern of the signals. 3 protons are giving three signals called as a triplet, 2 protons are giving 4 signals called as quartet. So this indicates the signal splitting which are taking place. So this simple NMR diagram explains the positions of these signals, intensity of these signals, type of protons which are present in this compound, so also the splitting pattern.

All this information can be obtained from the following references. 1. Organic Chemistry by R. T. Morrison and R. N. Boyd, 6<sup>th</sup> Edition, this gives basic idea about NMR spectroscopy. All the basic understanding with respect to NMR, how NMR is obtained? What are the simple compounds which can be easily studied by using this reference books where you can solve additional problems, try to gain more knowledge about NMR spectroscopy and using all these references and by studying different examples you can easily find out, or you can easily arrive at the correct structure of molecule which you are analyzing or which you are comparing.

Thank you.