Welcome to the module High Resolution Spectra in the unit molecular spectroscopy II of the Course CHC 108. In this particular module, we will be studying what is a high resolution spectrum. For that we should know what is a low resolution spectrum and also the difference between high and low resolution spectrum and will be also giving some examples which illustrate high and low resolution spectrum.

After learning this topic you will be able to get the difference between low and high resolution spectrum and you will be able to discuss the low and high resolution spectrum of some simple molecules.

Before understanding what is a high resolution spectrum, let us try to get some information about what is a lower resolution NMR spectrum. Now when we look at the NMR spectrum, the lower resolution NMR spectrum gives us the information about chemical shift of the hydrogen atom, that is it tells us in which atomic environment the hydrogen atom is present.This is one thing. Secondly, it gives us the height of the peaks, that is, the number of hydrogen atoms in the same environment. So when you look at the low resolution NMR spectrum, it looks very very simple. Now let us take the example of ethanol molecule.

Now Ethanol Molecule has got the structure CH_3CH_2OH so there are three protons on methyl carbon, there are two protons on methylene carbon and there is one proton on the hydroxy group. Now the low resolution NMR spectrum of this molecule will be as given in the figure where we can see that at the delta scale of 1.2 there is a peak which is due to methyl proton, that is the CH_3. Protons at the delta 3.63 we will have absorption due to the methylene protons, that is, the CH_2 protons and at delta 4.8 we will have the absorption because of hydroxy protons.OK so because all these three types of protons, they lie in three different environments, we get three peaks at different delta values. If we look at the height of the peaks, the height of the peaks are in the ratio of 3:2:1.So three is because three protons are absorbing, 2 is because two protons are absorbing and one because one hydroxy proton is absorbing.

So when we look at the low resolution spectrum, it gives us information about the chemical shift, that is the environment of the proton and it also gives us the height of the peak, that is the number of hydrogen atoms present in the same environment. Now. when we look at the high resolution spectrum, in the high resolution spectrum, which looks a bit complex, than the low resolution spectrum because in the high resolution spectrum there is the effect of spin spin coupling observed.

So in the low resolution spectrum we don't have the spin spin coupling.But when we look at the high resolution spectrum, there is spin spin coupling observed. Now the spin spin coupling happens between the protons which are on the adjacent carbon atoms and because of this spin spin coupling , there is splitting of the NMR peaks. That means the peaks we have seen in the earlier example, which was a single peak, now that single peak will split into many. The number of peaks obtained after splitting obeys n+1 rule, wherein n is the number of protons on the adjacent carbon atom. let's take a simple example.

Let's take the example of CH_2CH, OK, so here we see that in case of the protons that are present on the CH_2 carbon OK, and a proton present on the C carbon, we see that here the single proton that is present on this carbon atom will split its signal because of the two protons that are present on the adjacent carbon atom to it and by how much it will split, it is obeying the n+1 rule, so this particular proton will split itself. The signal of this particular proton will split itself because of two protons on the adjacent carbon atom, so it will become two plus one i. e., the signal will split into a triplet that is 3 peaks.

Similarly, when you look at the protons on this carbon atom, the protons on CH, these protons. They will split because of this single proton on the adjacent carbon atom and the splitting is again obeying n+1 rule which becomes 1 + 1 that is equal to two. So we get a doublet. The intensities of the split peak are given by Pascal's triangle, which is given below.

Now let's take the example of same ethanol molecule but high resolution spectrum.Now here we have to remember that ethanol molecule in a high resolution spectrum will show spin spin coupling.OK, so here we have the methylene protons, the methyl protons and the hydroxy protons. Now these methylene protons are adjacent to another carbon atom, which is having two protons, so here the methyl protons will split themselves into 2 + 1 equal to three peaks i.e. a triplet. Similarly the methylene protons are close to the methyl protons.OK, so the methylene protons will split their signal into 3 + 1 i.e. four i.e. a quartet, and if we look at the hydroxyl proton, this hydroxy proton shows a singlet because it doesn't couple with adjacent methylene protons, it undergoes continuous replacement.

It doesn't remain in the same environment for long for coupling to occur. So when we look at the high resolution spectrum of the same ethanol molecule, we get the peak due to methyl protons will now split into three peaks,the peak due to methylene protons will split into four peaks and the peak due to hydroxyl proton will remain same. So we will have triplet at delta 1.2 because ofCH_3 protons, quartet at delta 3.63 by CH_2 protons and the singlet at delta 4.8 by OH proton.

So here we have the difference between the low and high resolution spectrum of ethanol molecule, so here we can see how in the lower resolution spectrum we have got single peak and how in the high resolution spectrum the same single peaks have actually formed multiple peaks.

Let's take another example of acetaldehyde. So acetaldehyde molecule,the structure is as shown here.

It is CH_3CHO So when we look at the low resolution spectrum of this molecule, now we know that there are protons in two different environment. So we will have a peak at delta 2.2 because of methyl protons and another peak at delta 9.8 because of aldehydic proton. So the spectrum will look as given here. But when we come to high resolution spectrum of this same molecule we have on the adjacent carbon atom

the protons, so the CH_3 protons will split because of the CHO proton and the CHO proton will split because of the CH_3 protons. So in the high resolution spectra we will have the three protons splitting into n+1 plus one that is 1 + 1 equal to doublet as shown here and the aldehydic proton H splitting itself because of CH_3 that is the three protons.OK, according to the Formula n+1 it is 3+1=4. So the aldehydic proton will split the spectrum into a quartet. So here we see low resolution spectrum which is giving single peaks and high resolution Spectrum which gives multiple peaks because of spin spin coupling.

This is the book that has been referred while making this presentation.

Thank you.