One and Two Dimensional NMR Spectroscopy for Chemist

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Lecture - 38
Coupling among non-equivalent spins

Welcome back. In the last class, we extensively discussed carbon 13 NMR and I discussed how we are seeing the carbon 13 spectrum especially when it is directly attached to protons, the type of splitting we are going to see for a CH3 carbon, CH2 carbon, CH carbon; and also we saw what happened to the long-range couplings of carbon to protons, how it is going to be affected and we also saw that chemical shift of carbons are similar to the way the chemical shift to the protons are influencing proton chemicals shifts.

The way the proton chemicals shift are influenced by various factors, similarly the same factors affects the carbon 13 chemical shift. Most important thing I pointed out, because of the natural abundance of the carbon 13, it is not possible or practically it is impossible to see all the carbons in the molecule in carbon-13 state. As a consequence, we have different carbons in different carbon-13 states, corresponding to N chemically non-equivalent carbons in a molecule that is going to be N different isotopomers. As a consequence what you are going to see is the super position of this spectrum of each isotopomer. That is what I said, carbon 13 spectrum is a super position of the spectrum corresponding to each isotopomer. On the other hand, in the proton, I said it is spectrum of a single molecule. The carbon 13 spectrum is not from a single molecule it is super position of the spectra of N different isotopomers.

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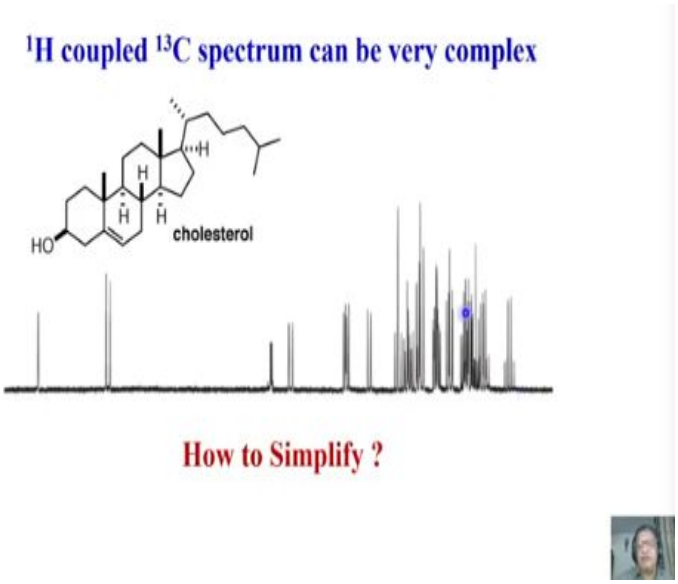

And finally we came to the situation, and saw the type of spectrum generally we observe for a molecule like this. But if I give you a spectrum like this the interpretation is as difficult as that of the proton spectrum. Understand, it is a really complex carbon spectrum similar to that of a proton spectrum. Now, how do you simplify?

See, first of all, the carbon 13 spectrum is always recorded with a decoupling mode. This is a proton coupled to carbon 13 spectrum, as I said this is a CH3 this carbon, this will be quartet, this will be quartet, this will be triplet, this will be triplet, this will be doublet, like that. So varieties of multiplicity pattern you are seeing. In fact, if you take a fully coupled carbon-13 spectrum there will be long range proton carbon couplings also, we cannot deny that. So everything is possible; as a consequence carbon spectrum is highly complex.

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Broadband proton decoupled, completely removes all the ^{1}H-^{13}C couplings

A single and distinct peak is detected for each chemically inequivalent ^{13}C

The question is, how do you simplify? The one way of simplifying the carbon spectrum is; generally carbon spectra are recorded with broadband proton decoupled mode. You see we always get a broadband proton decouple carbon 13 spectrum, what do you mean by broadband? That means for the entire range of carbon chemical shifts, we remove all protons that are coupled to carbon. This is called decoupling.

See completely broadband, entire range, we remove proton carbon couplings. As a consequence, what happens? no carbon is coupled to any protons. Understand no carbon is coupled to any of the protons. Then what will happen? Each carbon is going to give you a single peak. When we take the broadband decoupled spectrum of carbon; broadband decoupling means I am decoupling only protons, remember, carbon attached to all the protons I am removing. If it is attached to different nuclei, that is a different question, I am not removing that. That coupling will be there, that is what I said the beauty of NMR, only particular nuclei we can decouple.

Since these molecules, most of these molecules are organic molecules, protons will be invariably present attached to carbon, which is giving complexity for the spectrum. What we do is, we do at a time, remove all the couplings of protons with carbon. That is the best way, in which case you get 1peak for 1 carbon. What does it mean? If your molecule has 10 carbons, you get 10 peaks.

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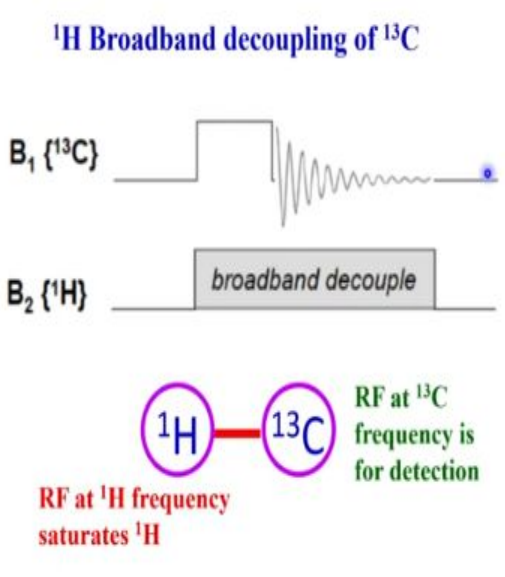

If your molecule has 6 carbons you get 6 peaks; that is all; very simple. So what you do in the case of the broadband decoupling carbon 13 is like this; see on the carbon 13, that is what we are detecting, I am going to apply radio frequency pulse and then start collecting the free induction decay. Apply radio frequency pulse on carbon and start collecting the free induction decay, and simultaneously, right from the beginning of the RF pulse, rf can be timed very properly, do not worry when I come to experimental set up I will discuss all those things, exactly at the point when you apply RF pulse, I can switch on decoupler, of the proton channel. There are different channels, modules in the NMR spectrometer. I am going to apply in the carbon 13 channel 90 degree pulse for detection; in the proton channel I am simultaneously applying relatively high power, so, that I will decouple all the protons with carbons.

How we do? this is what we do. At the proton frequency, at the center of the proton frequency, what is center of proton frequency? We know the proton chemical shifts 0 to 10 ppm or 15 ppm go to the center of that, let us say I take 0 to 10 ppm, at 5 ppm I am going to have an offset, that is called decoupler offset. I sit at the center of the proton spectrum and apply a radio frequency pulse.

Remember this is another radio frequency pulse, not this one; this is for detection. At the proton channel you apply another radio frequency pulse simultaneously with a high power and continuously; it is a continuous power we are applying, right from the beginning of the pulse till

the end of collection of the signal, i.e. FID, we keep applying the radio frequency and then we start applying the radio frequency here and start collecting the signal.

This is always on, see here in the figure, in the pulse sequence we can see power on the proton channel is always on right from the beginning till the end of collection of data, FID. Whereas carbon 13, we start collecting the signal simply apply 90 pulse start collecting the signal like you do routine 1D collection of the data, there is no problem at all.

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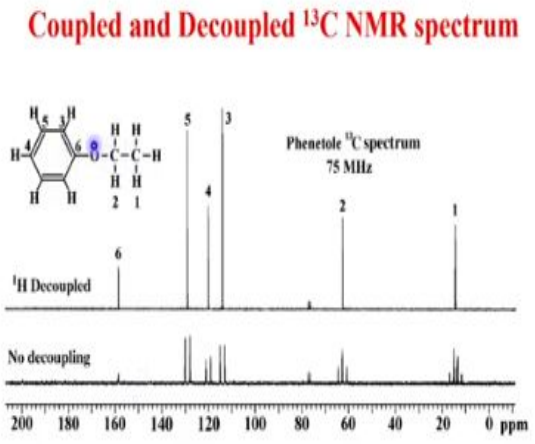

The question what happens in a decoupling everything I will explain to you when you come to decoupling. I will be discussing more about decoupling, when there is an opportunity, we will soon do that. And now we let us see what happens if I do the decoupling of carbon 13 spectrum. Take this molecule, it is called some Phenetole or something, it is at 75 megahertz when I take the carbon 13 spectrum.

This is what it is, very clear you all know that; this is a CH3 this one which comes at high field and this carbon is a quartet, you know why? because attached to three protons chemically equivalent. This CH2 is a triplet because it is attached to two protons, so it is a triplet and each of these aromatic carbon is a CH carbon, so it is directly attached with a proton, it is coupled to directly attached proton, each carbon is going to be a doublet.

And this quaternary carbon, carbon 6 is not coupled to anything, so it is a carbon which is not coupled to any of the protons, this gives a singlet.

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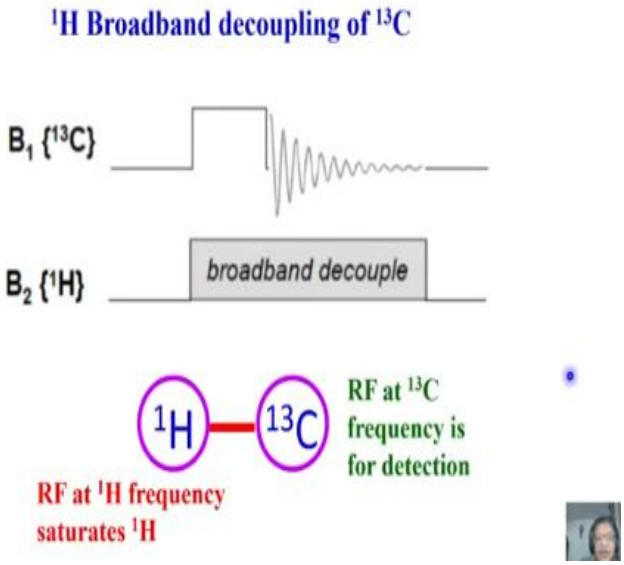

This is what it is, it is a spectrum, normal spectrum if you take the carbon 13 spectrum without doing any decoupling, it is only this part of this spectrum, bottom I am showing, this is not applied at all.

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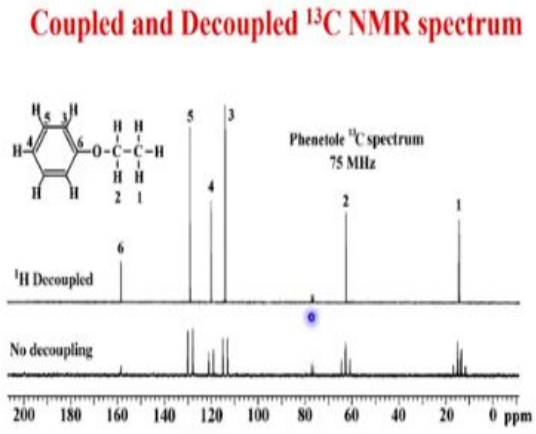

Now if I do the real decoupling, like this, while collecting the signal I also apply second radio frequency pulse at the proton frequency to saturate the protons, that means to decouple all the

protons coupled to carbons, and this is what we are going to get. Look at this what happened? The spectrum got significantly simplified. Look at this, these 4 peaks which were, there was a quartet, they all collapsed into a singlet because now it is not coupled to CH3 protons anymore.

There is no splitting of the energy levels; or no splitting of the peaks; they overlap, they collapse into a singlet, see now. Similarly, this triplet collapses into a singlet; all the doublets of the aromatic protons collapse into a singlet. Very, very interesting thing also happened. What is interesting thing? why it happened? Look at this one, all these signals intensity is much more now, because there is no more additional splitting. All of them collapse, the intensity will add up.

As a consequence, the signal to rise ratio becomes better. So, the advantage of taking decoupled carbon-13 NMR spectrum is the signal to noise ratio goes up, that is one thing; and the spectrum gets simplified; no more complexity. So you can directly count the number of peaks and start telling how many carbons are there in this molecule, simply look at this one, there is 1 carbon, 2 carbon, 3, 4, 5, 6, there are 6 peaks; you count the number of carbons, this 1 carbon, 2 carbon these two are identical because of symmetry; these 2 are identical; these two are identical; 4 and 5, and this carbon, total 6 carbons are there.

You may ask me the question what are these three lines? Why are they coming? This is because of CDCl3 that was used. This is CDCl3 where carbon is coupled to deuterium. In the proton, if it is not 100% deuterated you will get a peak residual peak, but here we are directly seeing the CDCl3; carbon which is directly attached to deuterium, carbon which is directly attached deuterium. Remember deuterium has spin one. As a consequence, each line of this carbon peak is split into 3 lines of equal intensity. You understand, this is a CDCl3 peak, coming because of carbon directly bonded to deuterium, which has spin one, and this carbon is split into 3 lines of equal intensity due to deuterium coupling. So this is way you get this solvent peak, do not worry we will come to that later.

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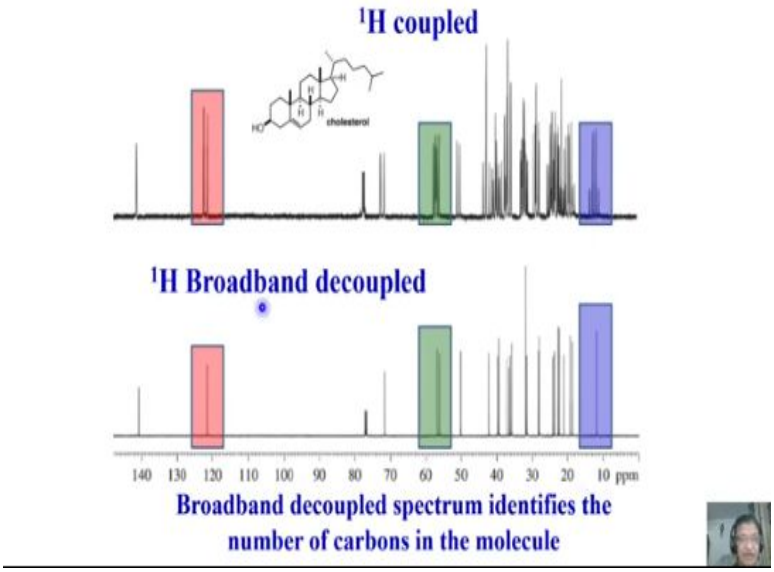

Now we let us go back to the cholesterol molecule, earlier we saw that, and this was the complexity of the spectrum which I showed. So this was the earlier one we saw, now we go back and see that spectrum and compare with the present spectrum, which is obtained with broadband decoupling. Continuous wave CW broadband decoupling. Look this quartet is collapsed into a singlet, this doublet collapse into a singlet, you see.

Now one or two I have highlighted just to get you clarity. See these four lines pattern 1,3,3,1 became a single line. And these 2 doublets, were there and it became only two singlets here; and this is again a doublet became a singlet. Look at the signal to noise ratio, look at the noise of this spectrum here. This is a noise, this noise is much more compared to here.

The signal to noise ratio is considerably improved in the broadband decoupled spectrum. You get this spectrum faster because you do not need to acquire more number of signals because the signal to noise ratio is quite high compared to this. This is the biggest advantage, not only it simplify this spectrum, signal to noise ratio is also better. As a consequence, you can get this spectrum faster. It does not take much time to get the good spectrum. That is the one important point.

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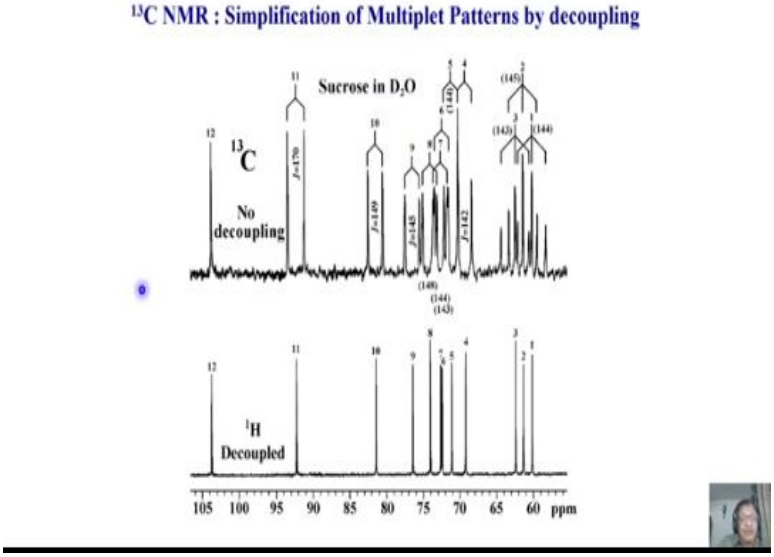

So as an example you can see how the complex multiplicity pattern sometimes are seen. In the previous example, you knew these are all are identifiable doublets, quartets. Consider a situation like this, here the triplet is overlapped it is not only identifiable triplets, one of the peak of triplet comes here, one of the peak comes here and this triplet peak comes here. Then they all crossover, there is an overlap, peaks are not clear identifiable, they completely crossed over to different regions. That is the case, how do you identify that? This is the spectrum of sucrose in water. In which case this spectrum complexity is difficult for us to identify which are the triplets, which are the quartets, which are the doublets? But decoupled spectrum easily we could identify the sucrose there are 12 carbons, we are observing only 12 peaks. Now the question I will ask you, what is happening to D2O peak? Why I am not seeing? I saw this solvent peak CDCl3. Remember in the previous example carbon was directly coupled to deuterium, deuterium is spin one, J coupling gave carbon three lines of equal intensity. But there is no carbon here, so when we use the D2O as a solvent in carbon 13 NMR you will not see any solvent peak at all, there is no residual solvent peak. Beauty is it not? Nothing is there, you get directly only peaks from your sample.

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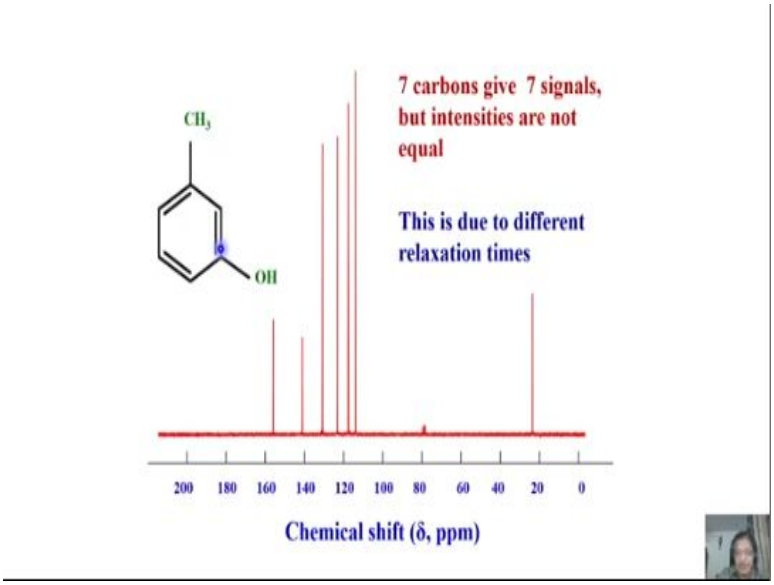

And seven carbons in this molecule gave me seven signals. I just want to tell you one interesting point, you count the number of carbons, there is no symmetry in the molecule, 1 carbon, 2, 3, 4, 5, 6, 7 carbons. You count seven peaks are there 2, 4, 5, 6, 7. But do you observe one difference here, why all the carbons are of not of equal intensity. If one carbon is there one peak, there are 7 carbon 7 peaks. Why there is a difference in the intensity of the peak? How do you understand that? This is another important point you must know. This is because different carbons have different relaxation times. So they relax, I will talk to you more about relaxation later, in fact we got an idea of it in one or two classes. First class I explained to you what happened to the FID, it relaxes back to Z axes with a spin lattice relaxation. Spins dephase in the XY plane due to spin-spin relaxation, T1 and T2 concepts I told you.

So how fast these signals from each of this carbon will come back to thermal equilibrium defines the relaxation time T1 and they are not same for all the carbons. They are different for different carbons for various reasons. The relaxation mechanism is different for each carbon. As a consequence, what happens? You will not get peaks of identical intensity. You can get it still. You know what you have to do? You have to do an experiment where in, when you start applying one pulse and collect the signal. If you want to keep on adding this signal, for signal averaging, for better signal to noise ratio. Before you apply a second pulse you have to wait for a

longer time. How much time? When I come to practical applications, practical difficulties of NMR according to NMR spectra in the practical aspects I will discuss those things;

The delay between one pulse you apply and then again second pulse, should be at least 5 times the largest T1 of a carbon peak, largest T1 of any carbon. That is, if this carbon relaxation time is five seconds, this has the relaxation time of let us 10 seconds, this has the relaxation time of let us say 20 seconds. Do not worry about 10 or 5, one which has largest relaxation time, the one carbon which takes more time to relax take that carbon.

You find out what is the relaxation times of all the carbons. And the one which has the longest relaxation time. this takes 20 seconds. 5 times at 20 second you have to take, 5 x 20, 100 seconds you have to take. And if you give the relaxation delay between the pulses, first apply a pulse, collect the signal, give a delay, again you apply the pulse, and collect the signal. You can do this co-adding of the signals; but then before you apply another pulse you have to wait for another 100 seconds.

If you do that, then all the carbons would have relaxed back to thermal equilibrium. Then you will get equal intensity. But normally we do not do that because it takes a lot of time. I tell you when the practical aspects we say what type of pulse we are applying and how much time we wait everything. As a consequence, you do not get peaks of equal intensities, otherwise we should expect peaks of equal intensity.

If you are very particular about these things you have to wait for 5 times the longest T1 of the particular spin in this molecule or particular carbon and then acquire the data.

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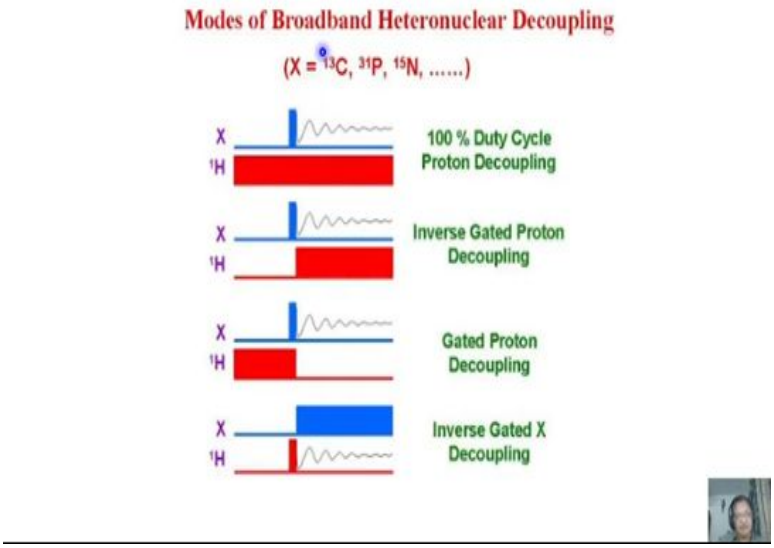

So the types of decoupling what we do? I said what we do in the case of decoupling is this. There are varieties of decoupling we can do. Remember in the experiment I showed, we applied the radio frequency pulse and started applying the RF pulse right from the pulse to end of the acquisition of the data. You can do many things. We can keep the decoupler power on, all the time here and the proton channel, even during the relaxation time here, and collect the signal.

Or I can switch off the decoupler time here and have the decoupler on only during the acquisition of the data. Or I can keep the decoupler on only during the relaxation time and switch it off during the acquisition of data. Or I can do one more thing, I do not switch on decoupling power for a long time and I apply only for a short duration. And another way I can do, inverse gated decoupling.

So there are varieties of ways of doing decoupling; this I will explain more later when I come to that. So there are several ways of doing this decoupling. In this case decoupling is on for a short time, and I am collecting the signal in the proton where I am decoupling the X nuclei. In all other cases decoupling power is applied on proton. This is the inverse gated decoupling, I will come to that later, we will explain each of these things now.

So there are several modes of doing broadband decoupling; and X means it need not be carbon. This experiment can be done for any heteronuclei. It can be phosphorous, it can be nitrogen

anything which is coupled to proton you can remove. Mind you in the present day spectrometers, it need not be only carbon you can detect while decoupling proton, you can detect phosphorus decouple carbon; verities of things are possible.

But this is for a chemistry people I am talking about carbon NMR, so basically we do broadband decoupling of protons.

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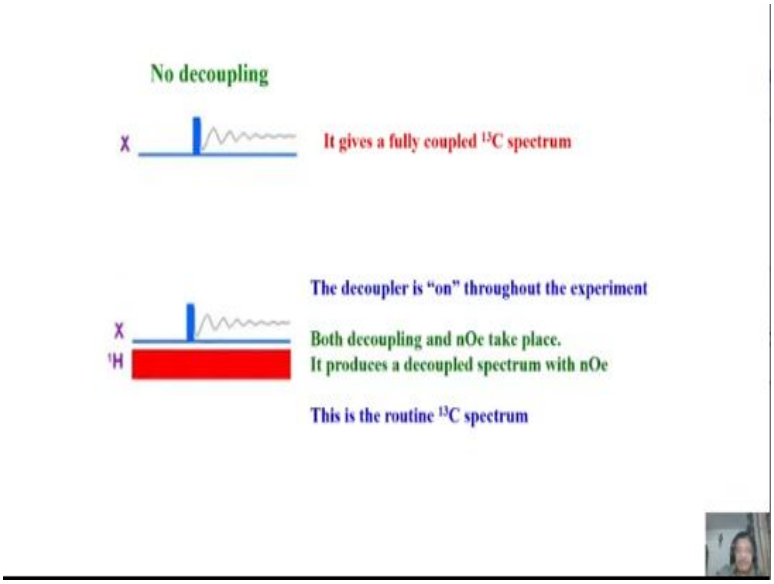

This is a situation, what will happen in this case? There is no decouple power on the proton channel at all, what does it give? It gives you fully coupled carbon 13 spectrum. There is no decoupling at all. Each carbon will be coupled to the protons attached to it and also remote protons, protons which are attached to carbons that are 2 bonds away, 3 bonds away. So it is called a fully coupled spectrum, no decoupling. It is a complex spectrum generally and signal to noise ratio is much less.

I can consider a situation like this with a decouple is on throughout the experiment. In this case what is happening is I will use the word called nOe; which next class or another one or two classes I will discussed more about nOe. Both decoupling and no nuclear Overhauser effect takes place in this case. It produces decouple spectrum with enhanced intensity.

What nOe does is, it will give you enhancement in the signal intensity. That is the point you remember till you understand nOe. When I do an experiment of broadband decoupling with nOe not only you get a decouple spectrum, you get enhanced intensity because you can increase the signal to noise ratio in addition to collapsing of the lines because of decoupling. There are two things happening, here decoupling will collapse the multiplets, I showed signal intensity goes up, signal to noise ratio goes up.

In addition to that another factor called nOe which adds to increased intensity. We will discuss nOe later and actually this is what you record in the routine carbon-13 NMR.

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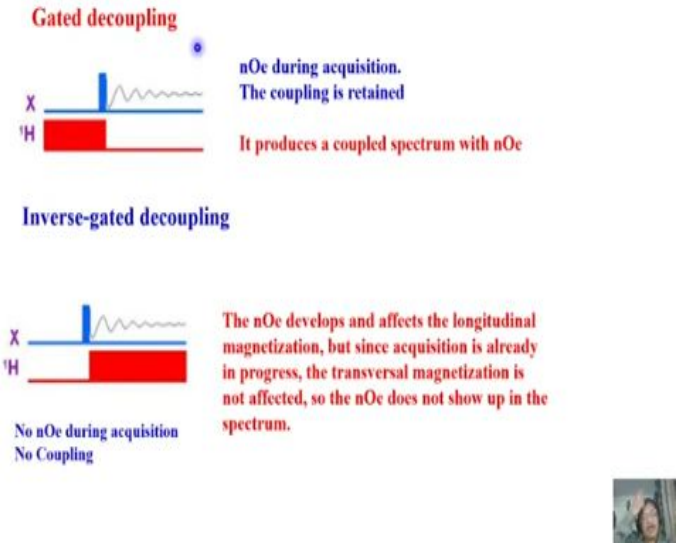

Another is called gated decoupling. What is gated decoupling is; I apply power only during the relaxation time and no power at the time of acquiring the data. See this is X nuclei, carbon. I am collecting the signal in the carbon channel and no decoupling is done at the time of acquiring signal. Only before the pulse I am applying RF power for proton channel.

It means there is nOe here; signal enhancement is there doing acquisition time; but at the same time coupling is retained. This is called coupled spectrum with nOe enhancement. We are going to get a spectrum with enhanced signal to noise ratio because of nOe plus coupled spectrum. This is what we going to observe. This is called gated decoupling. Also, we can do inverse gated decoupling that is also possible.

What we do is we apply a power, a pulse on the proton channel, do not apply any power at all; do not apply any RF power during relaxation time; and apply RF power only during acquisition. This means no nOe during acquisition and no coupling here. But here we are removing the coupling. So it is a decoupled spectrum without nOe, understand? This is a spectrum, nOe is not going to show up in this spectrum, but at the same time we are going to get the completely decoupled spectrum, no coupling at all.

The question is, this we have to discuss much more I have not talked to you about nOe everything, why nOe is not developed even though power is applied here? Ofcourse, there is a now that already the question has started; the transverse magnetization is not going to be affected here. As a consequence, nOe will not show up in this spectrum. nOe is an extensive discussion, I will do later.

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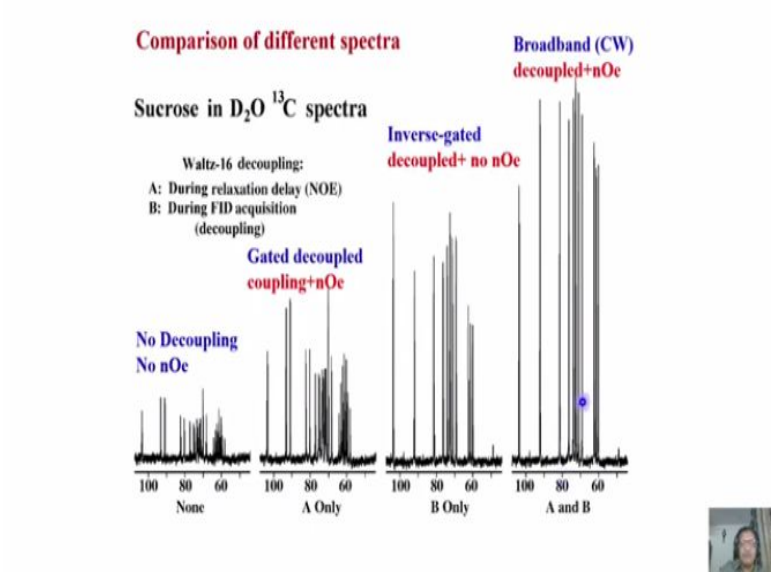

And now let us compare the spectrum, varieties of spectra of the molecule like this. The same sucrose molecule in D2O I took. This is a carbon 13 spectrum. Look at this, all the 4 experiments I am comparing, no decoupling, no nOe. What does it mean? There is no RF power in the proton channel at all. I am simply observing the signal, carbon 13 signal right? Send a RF pulse, 90 degree pulse, collect the free induction signal and detect the signal, no decoupling power at all.

But here, it is gated decoupled, that means there is a coupling plus nOe. This is inverse-gated decoupled, no nOe, this a broadband decoupled. That means decoupling plus nOe, both are present here. Look at the growth in the signal to noise ratio, as you go from one experiment to other experiment. You look at this signal to noise ratio, look at this one. What an enormous gain in signal to noise ratio. This is the experiment which we normally do. As a consequence of this type of experiment you will save lot of experimental time.

This spectrum if I have to take, carbon spectrum, it will take me one day and this will hardly take me half an hour. See the difference and this is what normally you have to do. So this gives you an idea of decoupling and what type of decoupling you have to do. Do not worry, simply remember you have to take broadband decouple spectrum with nOe. In a routine case, this is what we do. Nowadays, of course, you can do all those things with pulse sequences, I will tell you later.

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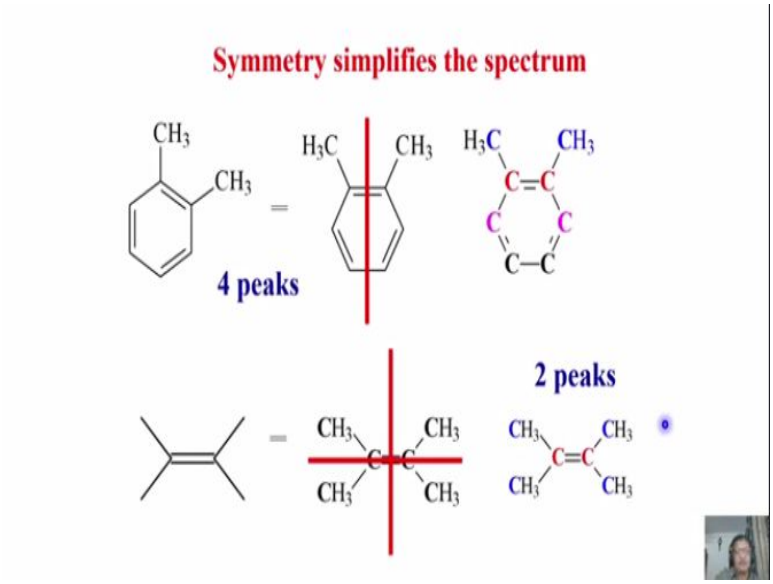

And of course, if I look at the carbon 13 spectrum, the number of peaks, again like in proton, if there is a symmetry in the molecule, the symmetry simplifies this spectrum. Look at this molecule, is there a symmetry axis? Of course, there is a symmetry axis along this. I just tilted the molecule later like this. And how many carbons are there in this molecule? This and this are equivalent, this carbon and this are equivalent, this and this are equivalent, this and this are equivalent.

So 1, 2, 3, 4 different types of carbons are possible here, 4 peaks you get, that is all. Look at this molecule. How many peaks I am going to get here? Only 2 types of carbons. This is all CH3s are equivalent and these two carbons are equivalent. As a consequence, you get only two peaks for this molecule.

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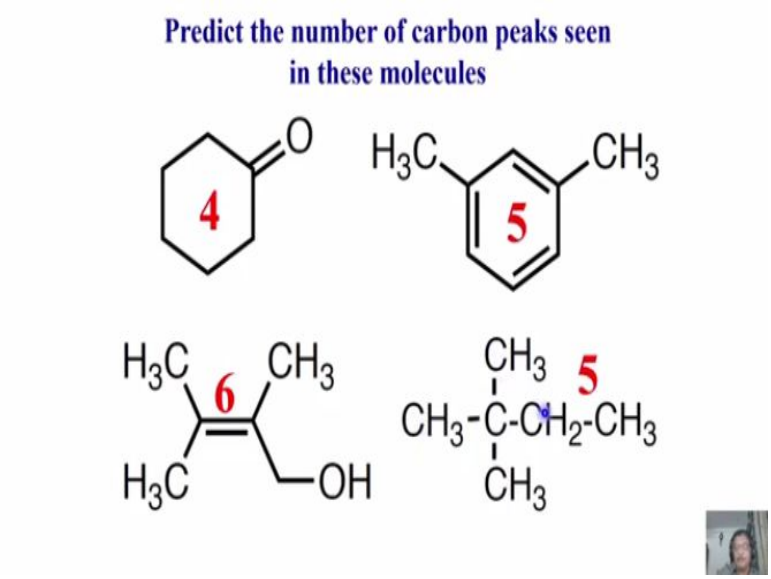

Now, we will predict the number of carbon peaks you see in these molecules. How many we can get in this molecule? Look at the carbons which are chemically equivalent. This is equivalent to, I assume there is a symmetry along this axis, there is a symmetry. This carbon is equivalent to this, this is equal to this; and this and this are different. So how many are there? There are 4 different carbons, you should get 4 peaks.

Now count for this, 1, these two are equal 1 carbon peak, this is different 2, these two are equivalent 3, this one is 4, where is the fifth one? This, 1, 2, 3, 4 and 5. You have to count this quaternary carbon also. What about this one? You simply count 1, 2, 3, 4, 5, 6. This one all are inequivalent here, there is no symmetry. No, there is symmetry I think. 1, 2, 3, 4 and 5, there are 5 carbons.

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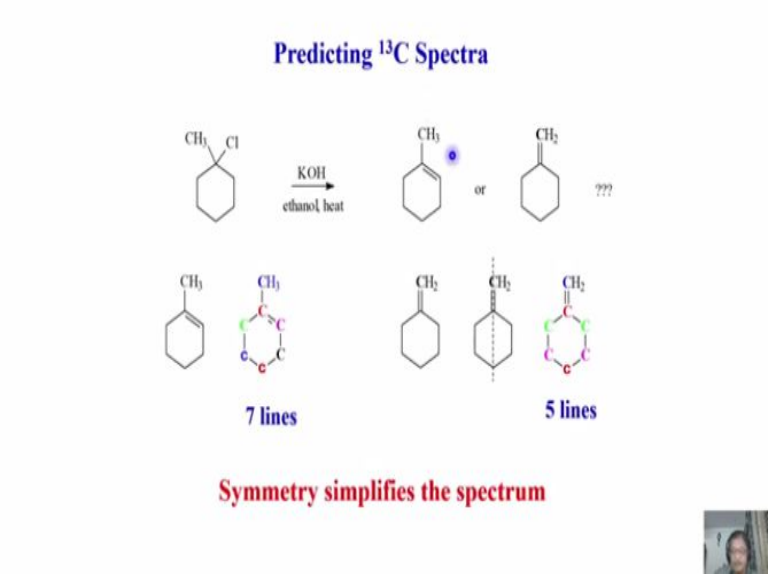

So you can use the carbon 13 spectrum to predict the reaction that takes place. Look at this molecule. Let us say, somebody is doing a reaction, what is the reaction let us not worry. Now the question is whether we got this product or this product. What is the answer? Let us assume I do not have proton NMR at all. I have to solve this problem only by carbon-13 NMR. How do I do that? Let us take the carbon 13 spectrum of it.

If this is my molecule, there is no symmetry here 1, 2, 3, 4, 5, 6, there are 7 lines. There are seven chemically in equivalent carbons, I must get 7 lines here. If this were to be my molecule, if that were to be the product, then there is a perfect symmetry along this, you should get 5 different carbons here; you get 5 lines. So carbon 13 NMR will identify which is your product, this or this, just because of symmetry considerations you look at the symmetry of this molecule, and then find out the number of peaks available or what you are going to get in the carbon-13 spectrum. Based on that you say this is the product or this is the product.

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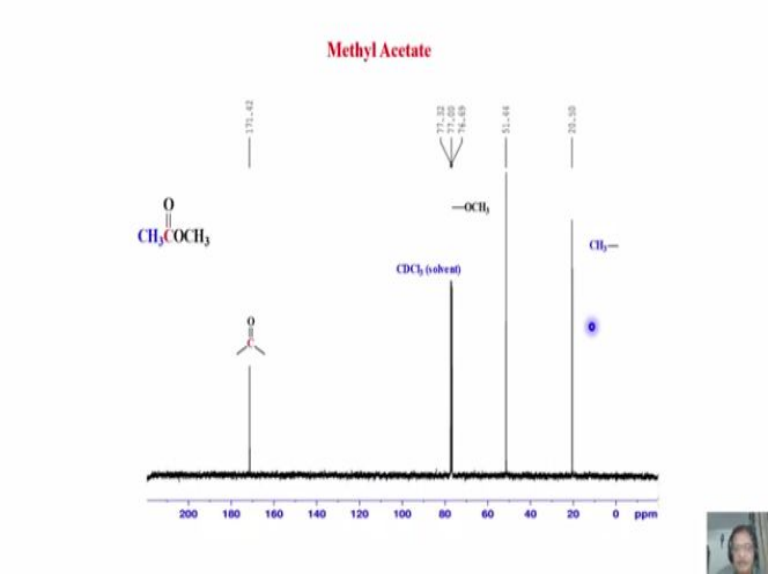

Now, let us start interpreting some of the simple carbon 13 spectrum. Acetone, it is the solvent which we normally use; this is the molecule. How many peaks you expect? CH3 carbon and CO carbon; there are only two carbons; one here and one here. Now, what is this? This is CDCl3 carbon coupled deuterium, spin 1, it is a 3 lines of equivalent intensity, here what is it.

What about this one, methyl acetate CH3COCH3? Now there is 1 type of carbon, CH3; other is OCH3 and 1 is CO carbon. So you expect 3 carbons, this is CDCl3, this is C double bond O. What about this one? It is OCH3 and this one CH3. So using the same like what you do for analysis of proton spectrum, same consideration depending upon electron negativity and you know which proton comes at high field. Similarly use the same logic and say which carbon comes at high field and then start making the assignments.

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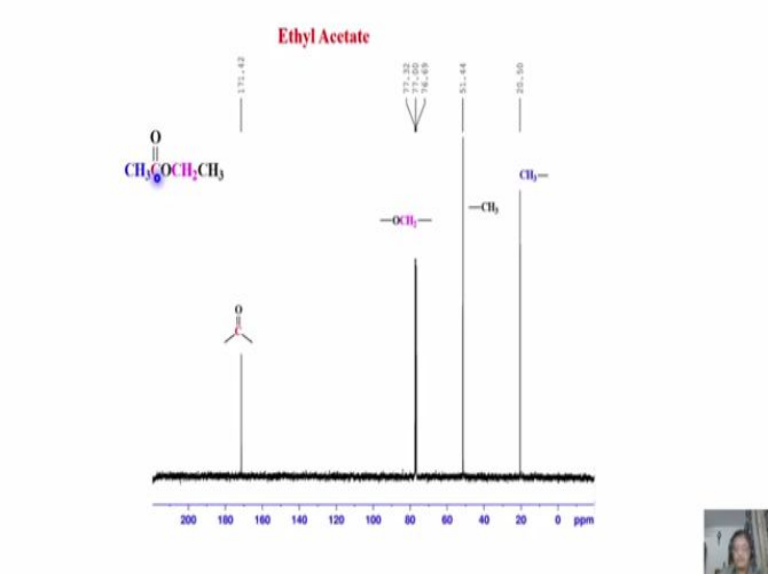

So this is ethyl acetate; how many equivalent carbons are there? you can see 1, 2, 3 and 4. Two CH3s, 1 CH2 and 1 CO. Look at this one, this is CO, this is OCH2, this one CH3 and this one CH3.

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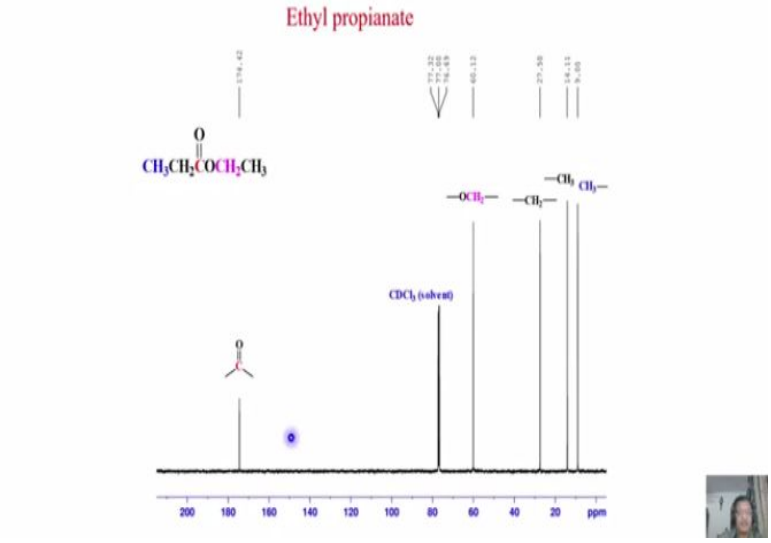

Now go to ethyl propionate. There are 1, 2, 3, 4, 5 carbons. Where are you seeing? See here, 1, 2, 3, 4, 5 carbons are here. 1, 2, 3, 4, 5 carbons are clearly visible, you can find out what are the CH3s. CH3s generally come at high field. This is CO carbon; this is a CH2 carbon, this is CH3 carbon, this is CH3 carbon, this is OCH2 carbon. Of course I know these 2 are CH3, this is CH2, this is OCH2, this is CO.

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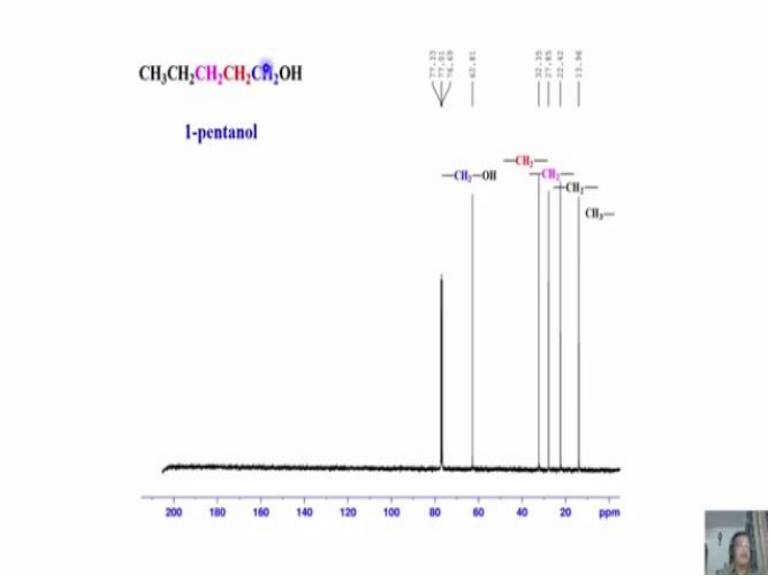

Very easily we can continue similarly for a molecule like this; we have 1, 2, 3, 4, 5 carbons, 5 different peaks are easily identified, CH3, CH2, CH2, CH2, OH. I know it comes down field. Now among the 3 protons here which is which? How to identify that? Which CH2 is this? How did I make this assignment? We will come to that, you can utilize the knowledge of the proton chemical shifts and then we can do that.

We will come to that later. We knew how to assign proton based on this triplet. This is a triplet, this is a quartet, this is a triplet of triplet. All those things we knew you know. Same way once you assign the proton spectrum, use the proton chemical shift knowledge and we can make the assignments of the carbon. We will do that when you come to do 2 dimensional HSQC spectrum.

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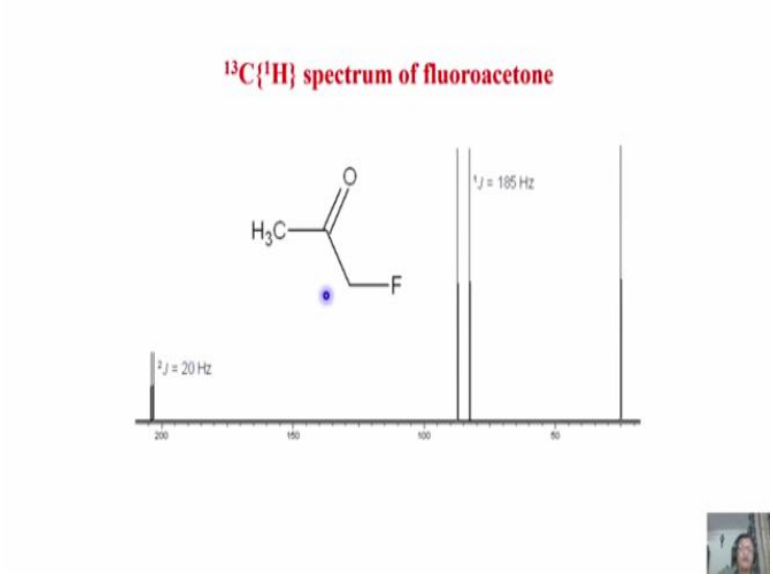

Now, this is a molecule; it is a fluoroacetone. One fluorine is present here and it is a proton decoupled spectrum. What does it mean? I decouple all the protons with carbons. Of course in the previous molecules also. These are all proton decoupled spectra. Here I am specially mentioning because remember, I am decoupling carbon with protons but not with fluorine.

Fluorine is still present, fluorine is coupled. So look at the carbon which is attached to proton this one. This has a large coupling, nearly 185 hertz is seen here and this carbon can also have a long range couple to this, this carbon; CO carbon. See long range fluorine carbon coupling of 20 hertz is there. Whereas this CH3, 1, 2, 3 bonds away, this coupling is very weak and is not seen. You are seeing only as a singlet because this carbon is coupled to only to proton that is removed because of decoupling.

So this CH3 is only a singlet and this directly attached carbon to fluorine is a doublet and this one is two bond coupled two bonds away, it is a doublet.

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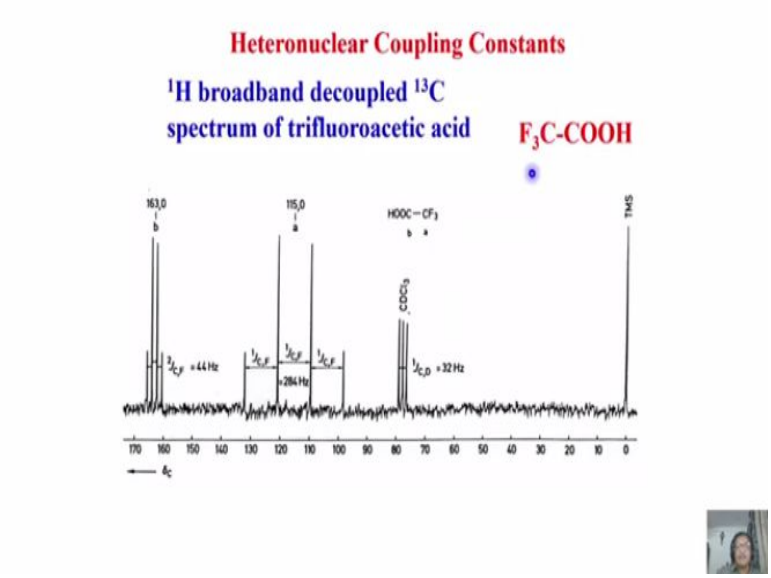

So we can keep on analyzing. I will analyze one simple carbon 13 spectrum with proton decoupling. Look at this molecule, proton decoupled carbon 13 spectrum of trifluoroacetic acid. We have to assign each and every peak here. First, of course, reference is TMS, no need to worry about it. What are these 3 peaks of nearly equal intensity? This is solvent peak, carbon-13 is coupled to deuterium spin 1, three lines of equal intensity, that also is well known.

Now the question is why this quartet and why this quartet? Remember this is CF3 carbon. This one bond CF3 carbon is very large and that is why this carbon is split into a quartet because of 3 fluorines. So it is a quartet, 1 3 3 1 intensity. CF3 carbon is a quartet and you are going to see this quartet. What about this carbon?

This carbon is having a long range coupling with three equivalent fluorines, long range coupling with this. As a consequence this carbon is split into a quartet because of these 3 fluorines. Please understand, now what is happening, many interesting information you can get here. Directly attached carbon to 3 equivalent fluorines gave a quartet. This is a 2 bond coupling, this carbon coupled to this three fluorines is going to be again a quartet, it is a long range two bond coupling which is 44 hertz, this is about 284 hertz.

Did you observe another interesting thing? If it was CH3, we expect this around 20 or 30 ppm. Whereas, CF3, look at it. It is coming around close to 115 ppm, why? Because it is attached to

electro negative fluorine. As a consequence there is enormous de shielding; as a consequence the CF3 group is coming downfield. So this how you can interpret carbon 13 spectrum but you may ask with a question what was a need for decoupling here, none of them are coupled to proton.

But in the COOH proton, it may have a long range coupling with this or this to ensure that it is broadband decoupled. So as a consequence there is no proton coupling here. So there is lot more we can talk about it. So today I will stop for the day. We have discussed a lot more about carbon-13 NMR which is one of the most extensively used nuclei, for all of you. Will come back tomorrow and continue little bit about carbon-13 NMR.

How do you assign the different carbons attached different protons etcetera by using certain techniques called DEPT, INEPT, APT etc. More discussion about that I will do later and then I will stop.