One and Two Dimensional NMR Spectroscopy for Chemists
Prof. N. Suryaprakash
NMR Research centre
Indian Institute of Science - Bengaluru

Lecture - 14
Conversion of Frequency and ppm

Welcome back, from the last 2 classes we have been discussing about one of the important NMR parameters, which is because of the internal interaction, that is chemical shift. We discussed several points about the chemical shift, but still we need to understand much more because it is one of the important parameters which is used when you want to analyze the NMR spectrum. The chemical shift and couplings are the parameters which you cannot avoid. So, it is better to spend a little bit more time to understand few things about chemical shifts, let us continue today with that.

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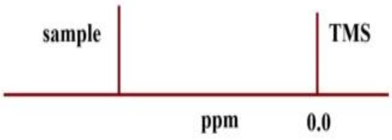
Reference

At different field, the resonating frequency varies. Thus chemical shift value is measured using a reference

For ^1H, ^{13}C and ^{29}Si, Tetramethylsilane (TMS) is used as the internal reference (set to zero frequency)



And last time I showed some spectra, and you know depending upon the symmetry of the molecule, how many peaks we can get and how can we get the integral area of the peak and identify the number of protons present in each peak everything. But when I say that different peaks are coming at different places, we must measure it, you know, what is it? there must be some reference, is it not?

If I start looking at for example, this peak, I say this is the frequency coming at some value, what is that value with respect to what? There must be some reference for everything. So, when you want to measure frequency, of course, without any reference also you can do it. But then I will say I measure the frequency and say this is 1000 Hertz, someone else an X, can go and record the spectrum in a different spectrometer. The different frequency spectrometer like I do it in 500, he does in 1000 mega Hertz, that he can say the same frequency. So, we need to understand with some reference, because different people can record the spectrum in the different spectrometer frequencies, and each may come out with a different value, it is not right. So, we must have a reference, generally for each nuclei which you want to take, like NMR of proton, carbon 13 or silicon 29, tin, lead any nuclei of your interest, there cannot be uniform reference for all the nuclei.

As a consequence, for different nuclei there are identified references, for example, for proton, carbon and silicon, tetramethylsilane is used as a reference. And the value of tetramethylsilane I know where it comes, generally it comes at a very, very high field. I will tell you why later, set that frequency as 0, with respect to that all other frequencies are measured. So tetramethylsilane is used as a reference for proton, carbon and silicon, for all the 3 nuclei, as a reference.

Of course, there are internal reference and external reference, tetramethylsilane is always used as an internal reference, very microscopic quantity, very minute quantity of TMS can be added to the sample and then take the spectrum, set this value to 0 and measure your frequency, that is normally what is done.

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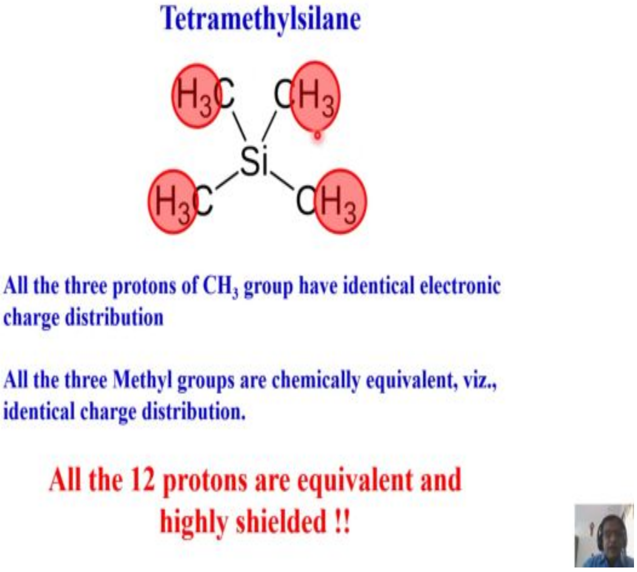

Tetramethylsilane

All the three protons of CH_3 group have identical electronic charge distribution

All the three Methyl groups are chemically equivalent, viz., identical charge distribution.

All the 12 protons are equivalent and highly shielded !!

And this is a tetramethylsilane, the question is, why are you using tetramethylsilane, why not something else? If you look at this molecule, this you can tetramethylsilane, this is a highly symmetric molecule all 4 CH3 groups are chemically equivalent. See this CH3, this CH3, this

CH3 and this CH3, all the 4 are equivalent. Of course, I have written this structure in a different way do not worry, but all chemist will definitely be looking at the molecule, they know what the structure and they know all this. Because of the symmetry all CH3 protons are chemically equivalent. In addition to that, protons within the methyl groups are also equivalent, very interesting is it not? See the chemical environment, electronic charge distribution at the site of CH3 and all these CH3 are same, identitical. All 12 protons are chemically equivalent with identical charge distribution surrounding them.

That means all 12 protons are equivalent, remember in the last class we found out the peak height, and then we say the number of protons are present, they like to do something, but individually I can say, if I take the protons spectrum of tetramethylsilane alone, because I know the molecular structure all are equivalent, I can say that there are 12 peaks in that. It is equal to all 12 protons are equivalent, very strong peak, but all 12 protons are resonating at the same place remember, as a consequence, if gives a very huge intense peak and only one peak, that is another thing.

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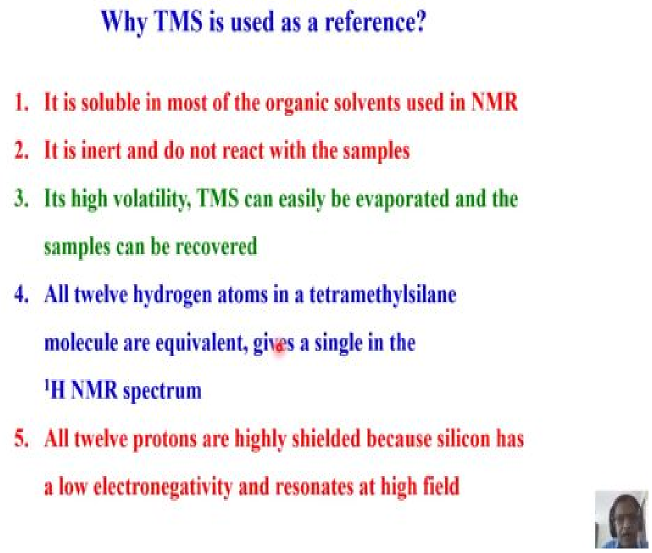

Why TMS is used as a reference?

1. It is soluble in most of the organic solvents used in NMR
2. It is inert and do not react with the samples
3. Its high volatility, TMS can easily be evaporated and the samples can be recovered
4. All twelve hydrogen atoms in a tetramethylsilane molecule are equivalent, gives a single in the ^1H NMR spectrum
5. All twelve protons are highly shielded because silicon has a low electronegativity and resonates at high field

The question is, so what, why should we use TMS as a reference? I know you can find some other molecule which has more protons and are chemical equivalent. I do not know if it is there really, why cannot you use that as a reference? Naturally, the question will come, and the pioneers in this area, have already done a lot of work, and then they have come up with the reason why tetramethylsilane, which is also called TMS is used as a reference?

First, it is soluble in most of the organic solvents used in NMR. So, what happens is when you want to study the solutions state of NMR, the molecule of your interest should be dissolved in the solvent, usually they are organic solvents like, chloroform, dimethylsulfoxide DMSO, acetone, CH3CN, acetonitrile, etc., these are deuterated solvents, I tell you why we have to use dueterated solvents in next 1 or 2 classes. But right now, you remember these are all organic solvents we use, and TMS is soluble in organic solvents.

Second important point, TMS is inert and do not react with the sample, it is inert, and if you say a sample of your interest you can be safe, your sample will not interact with TMS, there is no reaction that is going to take place. So, it is safe to use, secondly, it is highly volatile, it has a lot of volatility.

So, just open a TMS bottle in the laboratory keep it a big bottle of 100 ml within half an hour or so, you see the bottle will be empty. It will evaporate, it is highly volatile liquid. So as a consequence even if you add a small quantity of tetramethylsilane as a reference for your sample, since it is volatile and nonreactive with your sample, it is inert, simply you can evaporate out and you can recover your sample, very easily.

As I said in the previous slide, all 12 protons are equivalent, gives a single peak in NMR. Most important thing is all 12 protons are highly shielded, because silicon has low electronegativity and that is why TMS always resonates at a very high field. Most of the NMR spectrum of any molecule, of course, I am not telling all, most of them, there are some molecule whose spectra, comes beyond TMS also. If we take TMS as reference, but majority of the cases, all spectra will come below TMS, if we take TMS as 0 it comes less than TMS, More than TMS means higher field than TMS, less than TMS means less lower field than TMS. Sometimes you may come across some molecules, which can resonate beyond TMS even higher field then TMS, but, nevertheless, TMS is the best sample to use as a reference in proton, carbon and silicon, that is why it is widely used.

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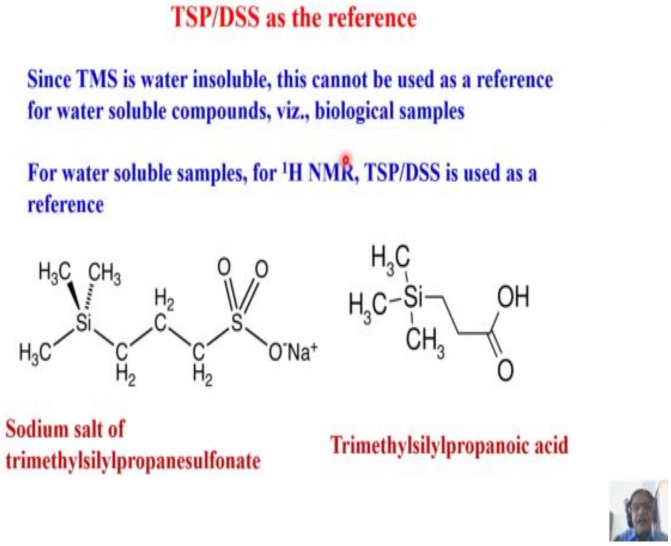

TSP/DSS as the reference

Since TMS is water insoluble, this cannot be used as a reference for water soluble compounds, viz., biological samples

For water soluble samples, for ^{1}H NMR, TSP/DSS is used as a reference

Sodium salt of trimethylsilylpropanesulfonate

Trimethylsilylpropanoic acid

I said, this is organic sample, you may ask me a question, what should I use, if I have to take proton NMR, where I have to study samples in non organic solvents? For example, I want to do in water, I have a biological sample, like a protein or peptide or something, which is soluble only in water, let us say. What to do? TMS is insoluble in water, some of the biological samples have to be studied only in water.

Then, what to do? In such cases for water soluble samples for proton NMR another reference used is called, TSP or DSS. TSP is tetramethylsilylpropanoic acid this is TSP. DSS is sodium salt of trimethylsilylpropanesulfonate, some big name, do not worry. Remember, for proton if you want to do in the water or any nonorganic solvent and especially a sample biological sample which is soluble only in water, reference cannot be TMS, reference has to be TSP or DSS.

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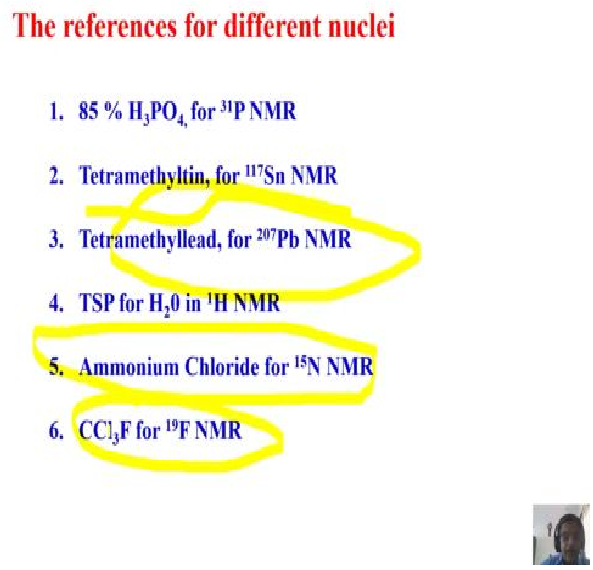

The references for different nuclei

1. 85 % H_3PO_4 for ^{31}P NMR
2. Tetramethyltin, for ^{117}Sn NMR
3. Tetramethyllead, for ^{207}Pb NMR
4. TSP for H_20 in ^1H NMR
5. Ammonium Chloride for ^{15}N NMR
6. CCl_3F for ^{19}F NMR

So, different nuclei have different references, as I told you. If you go back to this molecule, look at it, it has as a silicon, all carbons are equivalent, all protons are equivalent. So, only 3 nuclei are there in this molecule. All the 3 are NMR active. Interestingly, that is why TMS is used as a reference for NMR of all the 3 nuclei, but for different nuclei what you will do? if I have to look for, let us say phosphorus NMR, remember 85% H3PO4 is used.

That is important thing 85% of H3PO4 is used for phosphorus NMR, but tetramethyltin is used for tin NMR, again similar to TMS and 4 methyl groups are there, all the 4 methyl protons, and that is all 12 protons are equivalent. So, that is what is used for tin. If you come at lead NMR, see this is what, the tetramethyllead is going to be used. Of course, I said for TSP. For nitrogen 15 you are going to use what is called ammonium chloride, and fluorine NMR we use this one, CCl3F is what is used for fluorine NMR. E1

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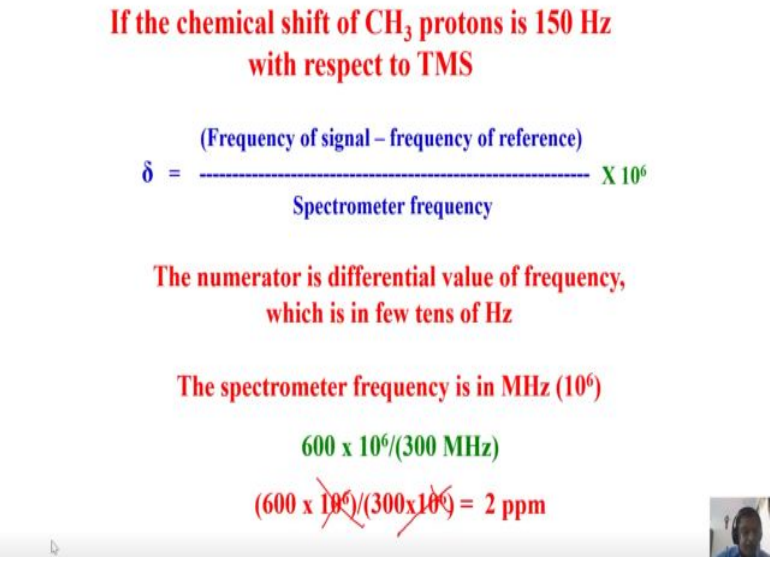

If the chemical shift of CH_3 protons is 150 Hz with respect to TMS

$$\delta = \frac{\text{(Frequency of signal – frequency of reference)}}{\text{Spectrometer frequency}} \times 10^6$$

The numerator is differential value of frequency, which is in few tens of Hz

The spectrometer frequency is in MHz (10^6)

$600 \times 10^6/(300\ \text{MHz})$

$(600 \times \cancel{10^6})/(300 \times \cancel{10^6}) = 2\ \text{ppm}$

So these are important things, but then when I say use as a reference, what is the reference you are using? We use TMS but, how do you measure this value? Remember the chemical shift of all the protons is expressed in what is called parts per million, delta, it is given as delta, delta is nothing but frequency of your signal minus frequency of your reference divided by the spectrometer frequency. Of course, multiplied by 10 to the power of 6.

I will tell you why we have to do this? You know the frequency of the signal with reference to the frequency of the reference. Let us say I am taking spectrum in 300 mega Hertz, 1 methyl group is there, only one methyl group, and TMS is there, both are coming at in 300 mega Hertz only spectrometer. But between TMS and methyl, the difference is very small. Both at 300 mega Hertz, a small chemical shift difference of the order of few 100 hertz, will be there.

So the difference in the frequency of the signal, with respect to the reference, is of the order of a few 100 Hertz. Whereas the spectrometer frequency is in mega Hertz, remeber. So, the numerator is in few hertz, the spectrometer frequency, the denominator is in megahertz, you should multiply that. Then for example, my chemical shift proton is let us say 600 hertz in a 300 megahertz spectrometer. The difference between the reference and signal is 600. And spectrometer frequency is, I said is 300 megahertz. So 600 divided by 300 into 10 to the power of 6, 300 megahertz, megahertz means 300 into 10 to the power 6. So you can remember remove this, and this and this will get canceled. You see for example, this will go and this will go. What is going to be left? 600 by 300, and you are going to get 2. So the chemical shift of CH3 protons, which is coming at 600 hertz in a 300 megahertz spectrometer is 2 ppm, remember this point, we express the chemical shift in ppm.

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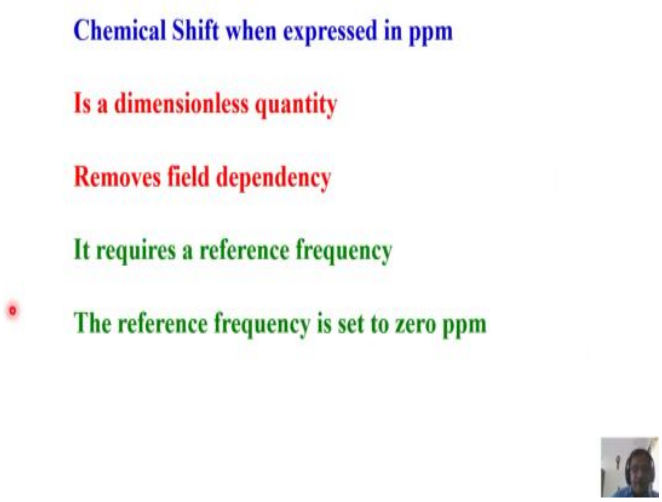

Chemical Shift when expressed in ppm

Is a dimensionless quantity

Removes field dependency

It requires a reference frequency

The reference frequency is set to zero ppm

So with this, let us see further, what is the advantage of expressing this chemical shift in ppm? Remember, when we express this chemical shift in ppm, interesting thing this is, ppm is a dimensionless quantity, there is a unit for it. If I say chemical shift of proton is 7 ppm, its 7 ppm, 7 parts per million, that is all. So whether you record in my spectrometer or your spectrometer, of different frequency, it does not matter, it is always same.

It removes field dependency, does not have any field dependency. That means let us say your chloroform comes at 7 ppm. In your 500 megahertz spectrometer, I am going to record in my 800 megahertz spectrometer. You say the chemical shift of chloroform is 7 ppm, I will also say 7 ppm. Because chemical shift, when expressed in ppm, there is no field dependency, it does not matter whichever the spectrometers we use, in whichever the field you study, the value is same, When expressed in ppm, it remains same. Remember that, and it requires a reference frequency, which we always use, and the reference frequency is set to 0. I already said the TMS.

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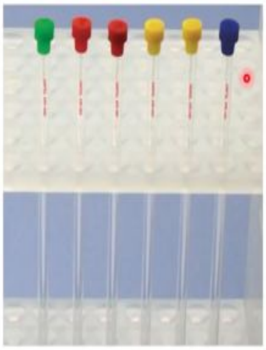
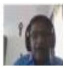
NMR in Solution State

The solute of interest should be dissolved in one of the deuterated solvents





So, generally when you want to take NMR in the solution state, this is what we do, just to show you. Go to any NMR laboratory and see what they are going to do. They take small, 5 millimeter tube of nearly 10 to 12 centimeter length like this, with different types of caps like this. Now, what you will do is, you will take the sample, put inside this along with your reference, and then put it in a magnet in the NMR spectrometer and record the NMR spectrum and the samples are always dissolved in the deuterated solvent. Remember that

If your sample is soluble in water, you cannot take H2O, you have to take D2O. If your sample is soluble in chloroform, do not take CHCL3, you must take CDCL3. You must always take deuterated solvent. Why you have to take deuterated solvent, what happens if I take CHCL3, a lot of information is available. I will tell you when you go to the parameters and the experimental conditions. How to record spectrum and all those things. These important things I will discuss later, but at the moment, remember, you have to dissolve this in the deuterated solvent. Put it in a 5 millimeter NMR tube of 10 to 12 centimeter length out it in a magnet and then start recording the spectrum.

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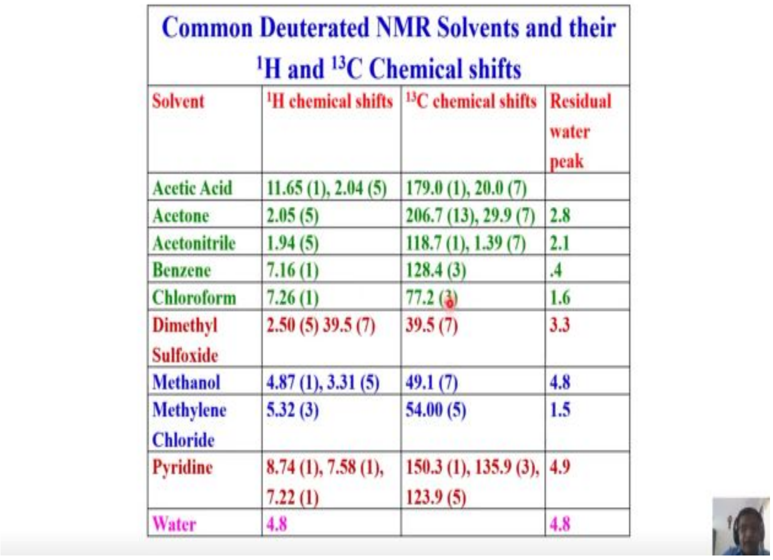

Common Deuterated NMR Solvents and their ^{1}H and ^{13}C Chemical shifts

Solvent	^{1}H chemical shifts	^{13}C chemical shifts	Residual water peak
Acetic Acid	11.65 (1), 2.04 (5)	179.0 (1), 20.0 (7)	
Acetone	2.05 (5)	206.7 (13), 29.9 (7)	2.8
Acetonitrile	1.94 (5)	118.7 (1), 1.39 (7)	2.1
Benzene	7.16 (1)	128.4 (3)	.4
Chloroform	7.26 (1)	77.2 (3)	1.6
Dimethyl Sulfoxide	2.50 (5) 39.5 (7)	39.5 (7)	3.3
Methanol	4.87 (1), 3.31 (5)	49.1 (7)	4.8
Methylene Chloride	5.32 (3)	54.00 (5)	1.5
Pyridine	8.74 (1), 7.58 (1), 7.22 (1)	150.3 (1), 135.9 (3), 123.9 (5)	4.9
Water	4.8		4.8

But, I said we need to take deuterated solvents, 100% deuteration is very difficult to get. always whenever you try to do there is some residual peak, residual water peak or residual protonated solvent peak, is always there. you cannot avoid that. Because I take, let us say, simple example benzene if I take 100% dueterated C6D6, can I get a proton NMR, is it possible to get proton NMR of benzene D6? No, because there are no protons.

You have replaced protons with deuterium, so you can get only deuterium NMR, proton NMR you cannot do. So, you must not get any signal if you take benzene D6, you should not get any peak from your solvent. But normally, it not does not happen like that, if you go and see the NMR spectrum, there is a benzene residual peak coming at 7.16, in bracket is an error 16 or 17 whatever it is, we can discuss that later.

So, this is the chemical shift of benzene, so, that means no solvent is 100% deuterated. There is always the residual protonated solvent present, that gives signal in proton NMR. You understand, similarly acetic acid CH3COOH, that means, it has a CH3 group and COOH group. There are 2 peaks for that protons. Otherwise, if you take CD3COOD 100% deuteration, there should not be any peak at all, same way in this list of solvents that I have given you, chloroform if we take, again it comes to 7.26, there is 1 peak.

And in addition to that if you look for carbon 13, these are all organic solvents, forget about D2O, H2O water, others are organic solvent, which also has carbon. Similarly, benzene has residual carbon peak, a proton peak here, but in the carbon what happens? You are not deuterating carbon, you are deuterating only the proton, so carbon is still there. So, carbon NMR is possible to record.

So do not get confused, this a residual peak, but this is not a residual peak, it is a peak from the solvent, it is present, and directly you can detect that. So all these solvents also has carbon peaks in the carbon NMR. For example, acetone, what is acetone? CH3 twice CO so you have CO peak here and CH3 peak here, both are present. See this is what happens if you look at this.

When it methanol, CH3OH, there are 2 protons signals, one for OH and one for CH3 and in carbon, you only have CH3 carbon, OH does not have any carbon, so that does not give spectrum in the carbon 13 NMR. So, these are all list of solvents, where you can see the residual protonated solvent peak and when you go for the carbon NMR, directly you get carbon peak.

Sometimes, what is going to happen is, when you record the spectrum, the solvents what you take may not be 100% pure, there will be always a residual proton peak, for various reasons. You want to try to put a solvent into your NMR tube, it may be hydroscopic. It will absorb moisture from your solvent. it is more so, especially in dimethyl sulfoxide which is highly hydroscopic and such solvents, because it has residual water, monomeric water will be there and that gives rise to residual water peak like this. For example in DMSO, if you find a peak in a NMR spectrum is taken in this solvent, at 3.3 it may be found in from your sample. But if you say I cannot expect the peak from my sample at this ppm, it could be residual water. Please remember, while interpreting the spectrum, this chart is very important. In addition to residual protonated solvent peaks, you will also get residual monomeric water peaks.

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Chemical Shift Range of ^{1}H Spectrum

TMS is referenced at zero ppm

Now, what is the range of chemical shift of proton? see I can measure the chemical shift with respect to tetramethylsilane which is set at 0 ppm. Different, nuclei have different chemical shift range. Generally, most of the cases in proton, the range is 0 to 10 to 12 ppm or in extreme cases 15 ppm. And all your peaks for most of your molecules, when you take NMR spectrum, measured with respect to TMS, will be within this range 0 to 10 or 12, 15 ppm.

In extreme cases, the proton attached to a metal or some extraordinary cases, it can go even below 70, 80 ppm. In extreme cases you can go even beyond TMS, even higher field at - 4, -5 ppm also peaks can come. There are exceptions. I am not telling as a rule that it has to come between 0 to 12 or 15 ppm. Remember, for majority of the molecules, the range of chemical shift of proton is 0 to 10 or 15 ppm, with TMS as a reference that you should remember.

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PPM to frequency, and frequency to ppm conversion

Now, one important thing you should know, always we express chemical shift in ppm and then we can find out the frequency of it. You can convert ppm to frequency, if I give the frequency of the peak in a particular spectrometer, I can convert it to ppm. If you give me frequency value, then you must also tell me the spectometer frequency. You cannot just like that say, Hai at 1000 Hz, or 2500 hertz I got a peak, tell me its ppm.

No, I cannot say, you must tell me what is the spectrometer in which you recorded the spectrum. Then I can convert frequency to ppm. Similarly, I know the water peak comes at 4.8 ppm, does not matter in whatever the frequency spectrometer, you tell me the spectrometer, I tell you what the frequency at which water peak comes. You understand the point, so ppm to frequency and frequency to ppm conversion is very, very important.

Please remember, because most of the time, people make lots of mistakes and they come to me. They do not know how to convert ppm to frequency and frequency to ppm, this is because, they are not exposed to it. So we should understand how to do that.

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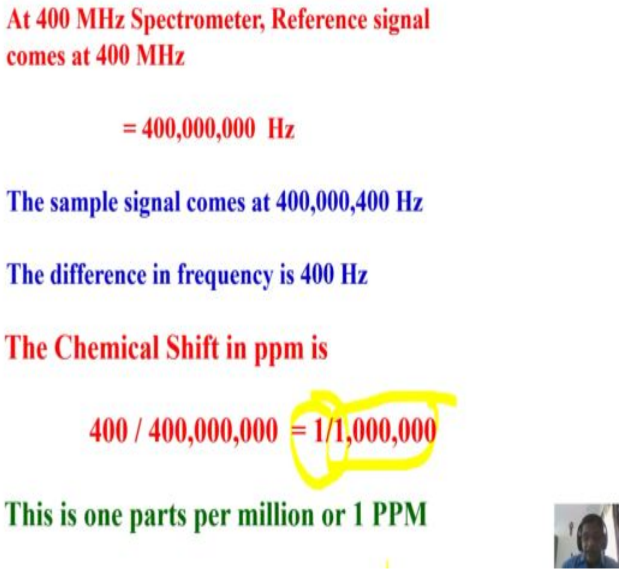

At 400 MHz Spectrometer, Reference signal comes at 400 MHz

= 400,000,000 Hz

The sample signal comes at 400,000,400 Hz

The difference in frequency is 400 Hz

The Chemical Shift in ppm is

400 / 400,000,000 = 1/1,000,000

This is one parts per million or 1 PPM

Now I will give you an example, at 400 megahertz spectrometer, reference signal comes at 400 megahertz, reference is TMS, fine. My sample I have, let us say, CH3OH or CH3CN, only one proton is there, one particular type of proton CH3 proton. Let us say it comes at 400 so many zeros, 400 hertz. Take the difference between these 2, 400 megahertz plus 400 hertz here, take the difference.

What is the frequency of my sample? It is 400 hertz. The difference is very small. We saw that you know when you wanted to measure the ppm, your sample frequency, minus the reference frequency, both are in megahertz, but the difference is in Hertz. That is what I said. Now the difference in frequency is only 400 hertz. Now, I said divide this by spectrometer frequency, that is one over 400 in a 400 megahertz spectrometer, that is one over 1 million, or this is 1 parts per million, 1 ppm.

How do you write this? If I have to write it I have to write as .000001, that is point five zeros one. That is cumbersome process, why we have to do that. For that purpose we simply ave to express this as a simple number without getting into so many decimal zeros, etc. Multiply these by 10 to the power of 6, then this will go, you will be left with only one, that is why we say it is 1 ppm. Are you understanding me do not get confused.

Now I am expressing the chemical shift in ppm; that is the difference in the frequency as 400 hertz divided by the spectrometer frequency 400 megahertz. It is one over one megahertz or when I multiply this by another 10 power of 6, this will go. And finally what you are going to see, remember this portion will go, when I multiply by 10 power of 6 and left it with only one here and that is my ppm. So ppm value is easy to express.

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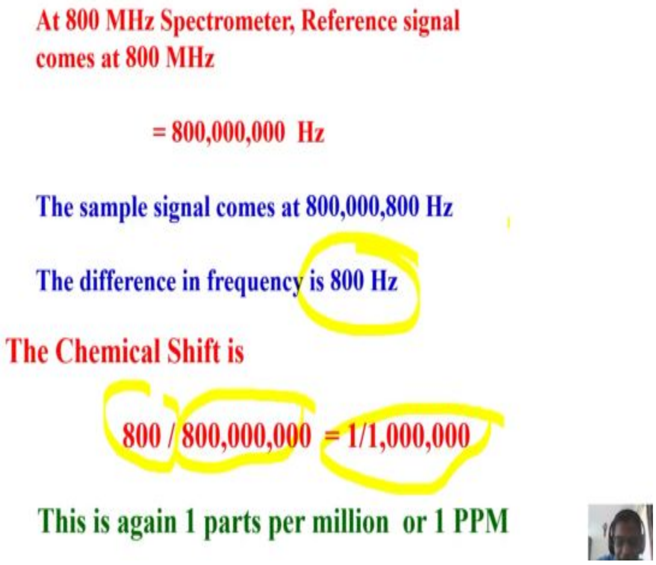

At 800 MHz Spectrometer, Reference signal comes at 800 MHz

= 800,000,000 Hz

The sample signal comes at 800,000,800 Hz

The difference in frequency is 800 Hz

The Chemical Shift is

800 / 800,000,000 = 1/1,000,000

This is again 1 parts per million or 1 PPM

Now at the 800 megahertz spectrometer, same peak, let us say, reference signal comes at 800 megahertz and sample comes by 8 megahertz plus 800. This is at 800 megahertz, and this is at 800 megahertz plus 800 here. What is the difference? 800 hertz. Now, calculate the chemical shift, 800 divided by 800 megahertz, it turns out to be again, one over one megahertz. As I said, multiply by 10 power 6, all zeros will go, we will be left with 1.

What does it mean? The same CH3CN I recorded at 400 megahertz, I got 1 ppm, I record at a 800 megahertz is 1 ppm. But frequency difference was 800 here, and 400 there, understand the difference. Here, with respect to reference it is separated by 800 hertz, my peak. In 400 megahertz with respect to TMS, it is separated by 400 hertz, when I converted to ppm it is same. ppm value remains same when expressed in ppm.

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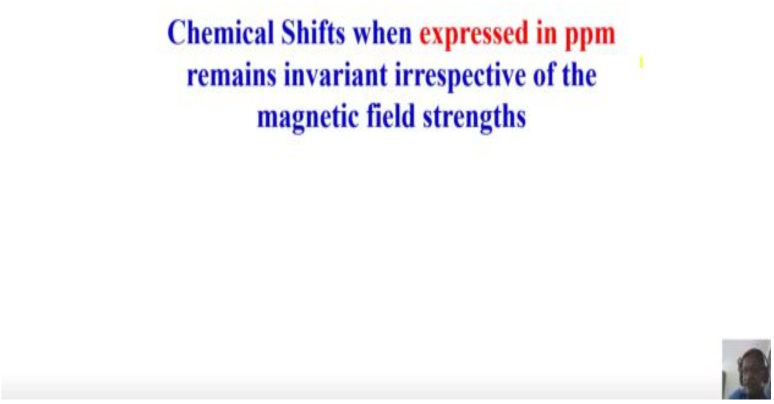

Chemical Shifts when expressed in ppm remains invariant irrespective of the magnetic field strengths

The chemical shift values when expressed in ppm remains invariant with respect to magnetic field. Whatever may be the magnetic field record the spectrum, when expressed in ppm, I do not care what the spectrometer frequency is. The value is constant, understood. Now, if I say benzene comes at 7 ppm at 400 megahertz, in 800 megahertz also it comes at 7 ppm but in frequency is different, just now we saw.

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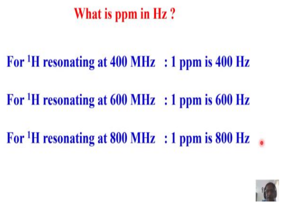

What is ppm in Hz ?

For ^{1}H resonating at 400 MHz : 1 ppm is 400 Hz

For ^{1}H resonating at 600 MHz : 1 ppm is 600 Hz

For ^{1}H resonating at 800 MHz : 1 ppm is 800 Hz

So, now we will try to understand what is a ppm? And what is frequency? What is ppm in hertz? Just now we saw for resonating frequency of protons coming at, let us say 400 megahertz spectrometer, 1 ppm is 400 hertz, just now we calculated that. Please remember, Just now we calculated 1 ppm is 400 hertz. Same at 600 megahertz, 600 hertz is 1 ppm. In

800 megahertz spectrometer 1 ppm is 800 hertz, very easy, when you want to express ppm in hertz, simply know the resonating frequency of that spectrometer, simply divide by that. See for example in 400 megahertz 1 ppm is 400 Hz, in 600 megahertz 1 ppm is 600, like that you can do.

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^{13}C has 4 times lower γ

Hence its resonating frequency is four times less than that of proton

^{13}C resonates at 100 MHz : 1 ppm is 100 Hz
(In a 400 MHz instrument)

^{13}C resonates at 150 MHz : 1 ppm is 150 Hz
(In a 600 MHz instrument)

^{13}C resonates at 200 MHz : 1 ppm is 200 Hz
(In a 800 MHz instrument)

Now, carbon 13 if you do in the same spectrometer what happens? Carbon 13 has gamma 4 times less, in the same spectrometer 400 megahertz of protons, carbon comes at 100 megahertz. Then what is a 1 ppm of carbon? remember it is not 400 Hz, it is 100 hertz because the resonating frequency of carbon is 100 MHz, whereas that of proton is 400 MHz. So, for proton 400 Hz is 1 ppm, whereas, for carbon 1 ppm is 100 hertz.

Similarly, at 600 megahertz carbon comes at 150 MHz, 1 ppm is 150 hertz, same way carbon resonates at 200 megahertz in a 800 megahertz spectrometer 1 ppm in proton is 800 Hz, whereas, for carbon 13 in the same spectrometer, 1 ppm is 200 hertz.

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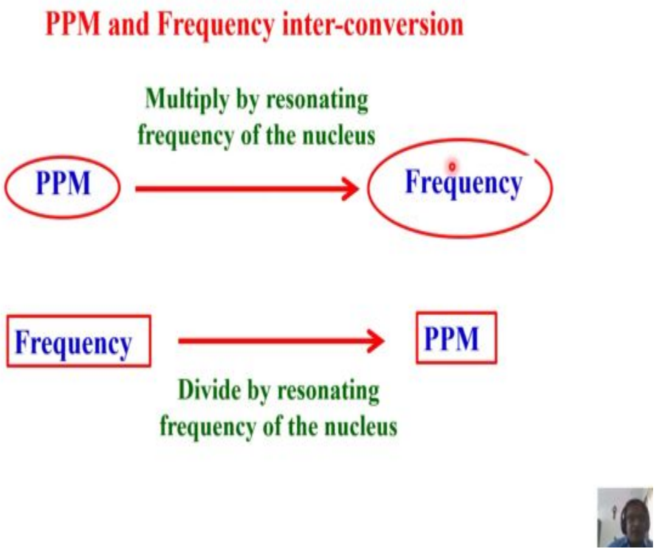

PPM and Frequency inter-conversion

Multiply by resonating frequency of the nucleus

PPM → Frequency

Frequency → PPM

Divide by resonating frequency of the nucleus

You understood the point now, ppm to frequency conversion and inter conversion we have to do like this. What you do is, for ppm if you want to convert to frequency you simply multiply by the resonating frequency of the nucleus. Remember this point if I want to know ppm, if I have to convert it to frequency ,multiply by resonating frequency, let us say I have chemical shift of 7 ppm of chloroform, in 400 megahertz, it is 7 into 400, 2800 hertz.

The same 7 ppm in 1000 megahertz 7 into 10, so, it is 7000. So, like that you should remember how to convert ppm to frequency. For ppm to frequency conversion, you have to multiply by the resonating frequency of the nucleus.

Now, for converse what to do? If you want to convert frequency to ppm, simply divide by the resonating frequency. If I say the resonating frequency, I got is 2500 in a 500 megahertz spectrometer, what is it in ppm? 2500 divided by 500, how much? 5 ppm. you understood the logic, so simply this is the important point you must remember this is what most of the people who come to me have made mistakes. Do not make mistake, please remember, for ppm to frequency conversion you have to multiply by the resonating frequency, for frequency to ppm you have to divide by the resonating frequency.

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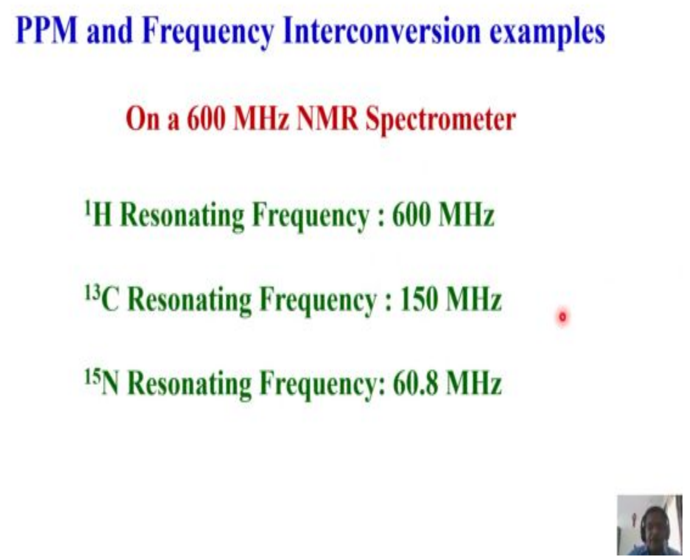

PPM and Frequency Interconversion examples

On a 600 MHz NMR Spectrometer

^{1}H Resonating Frequency : 600 MHz

^{13}C Resonating Frequency : 150 MHz

^{15}N Resonating Frequency: 60.8 MHz

We can do, number of such examples of ppm and frequency inter conversion. I will give you 1 or 2 examples today, before stopping. On a 600 megahertz spectrometer, proton resonates at 600 MHz, carbon resonates at 150 MHz, Nitrogen resonates at 60.8 MHz; why? we have been discussing because gammas are different. This gamma is almost 4 times smaller, This is almost 10 times smaller. In the same spectrometer of 600 megahertz, proton comes at 600 MHz, carbon comes at 150 MHz, nitrogen comes at 60 MHz, remember this point.

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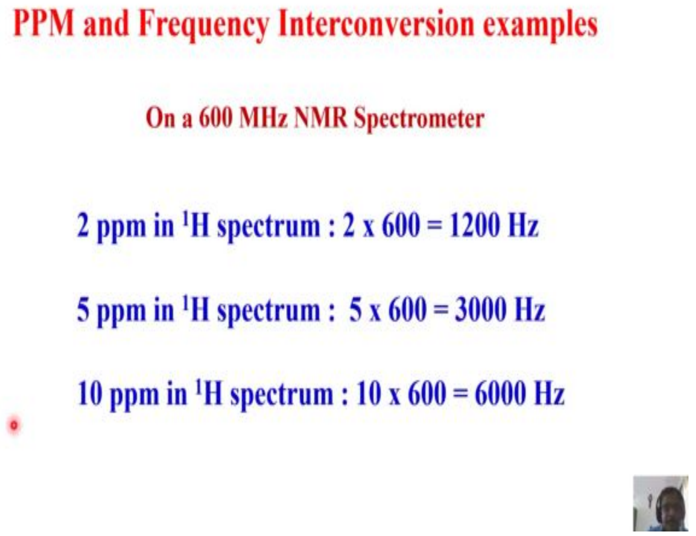

PPM and Frequency Interconversion examples

On a 600 MHz NMR Spectrometer

2 ppm in ^{1}H spectrum : $2 \times 600 = 1200$ Hz

5 ppm in ^{1}H spectrum : $5 \times 600 = 3000$ Hz

10 ppm in ^{1}H spectrum : $10 \times 600 = 6000$ Hz

Now, I will ask you a question what is 2 ppm proton? 2 into 600 ,you have to multiply by frequency to convert ppm to frequency. it is 1200 hertz; are you all with me? Now I want to convert 5 ppm of proton to frequency, 5 ppm in 600 megahertz is 5 into 600, 3000. similarly 10 ppm is 6000 hertz.

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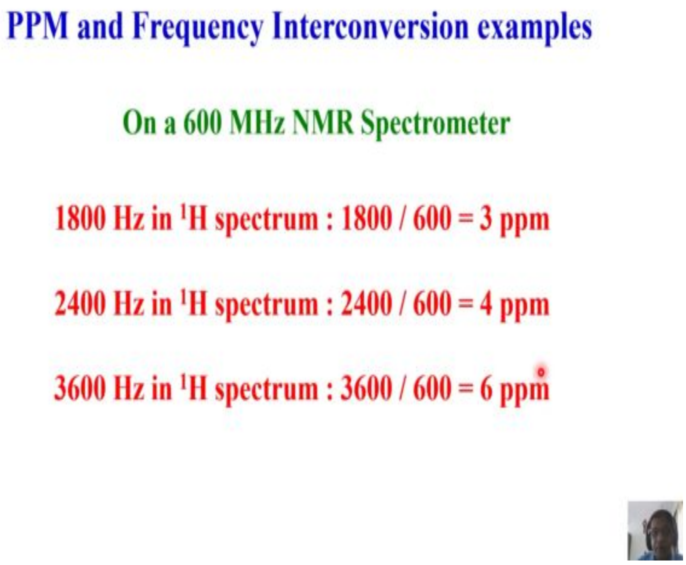

PPM and Frequency Interconversion examples

On a 600 MHz NMR Spectrometer

1800 Hz in ^{1}H spectrum : 1800 / 600 = 3 ppm

2400 Hz in ^{1}H spectrum : 2400 / 600 = 4 ppm

3600 Hz in ^{1}H spectrum : 3600 / 600 = 6 ppm

Now, on a same 600 megahertz spectrometer I have a peak at 1800 hertz. How many ppm is this? Divide by 600 it is 3 ppm. Similarly, at 2400 hertz I have a peak, divide by 600 will get 4 ppm. At 3600 hertz if you have a peak, divide by 600, you have a peak at 6 ppm. So this is the way you can convert ppm and frequency. From the inter conversion is possible to say. These are all important things to understand how to convert ppm into frequency, and etc.

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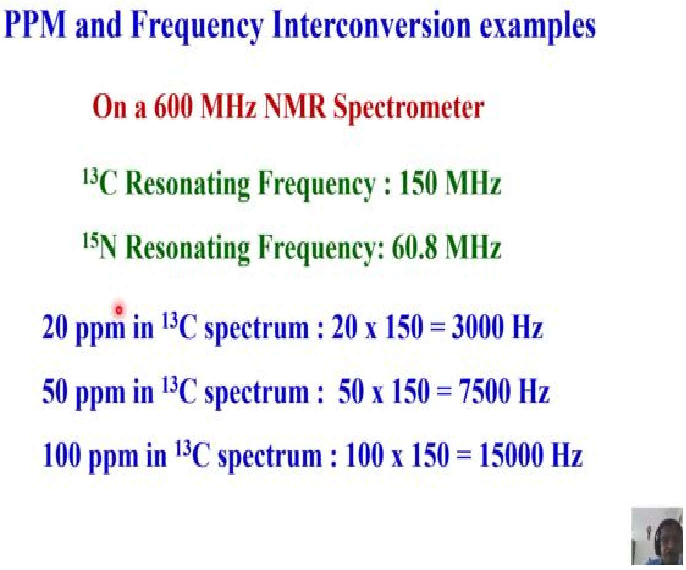

PPM and Frequency Interconversion examples

On a 600 MHz NMR Spectrometer

^{13}C Resonating Frequency : 150 MHz

^{15}N Resonating Frequency: 60.8 MHz

20 ppm in ^{13}C spectrum : 20 x 150 = 3000 Hz

50 ppm in ^{13}C spectrum : 50 x 150 = 7500 Hz

100 ppm in ^{13}C spectrum : 100 x 150 = 15000 Hz

Now, I will take another simple example. On a 600 megahertz spectrometer carbon comes at 150 Mhz. Now, what is 20 ppm in carbon here? Remember now, it is 150 megahertz in the same 600 spectrometer. So, 20 ppm in carbon is 20 into 150, do not multiply by 600 now, do not get confused, that was for the proton. Now the carbon resonating frequency is 150, so 20 ppm of carbon is 20 into 150, 3000 hertz, fairly simple right? Do not get confused, do not make mistakes. Please remember this 50 ppm, 50 into 150, 7500 hertz, same 100 ppm of carbon 100 into 150, 15000 hertz.

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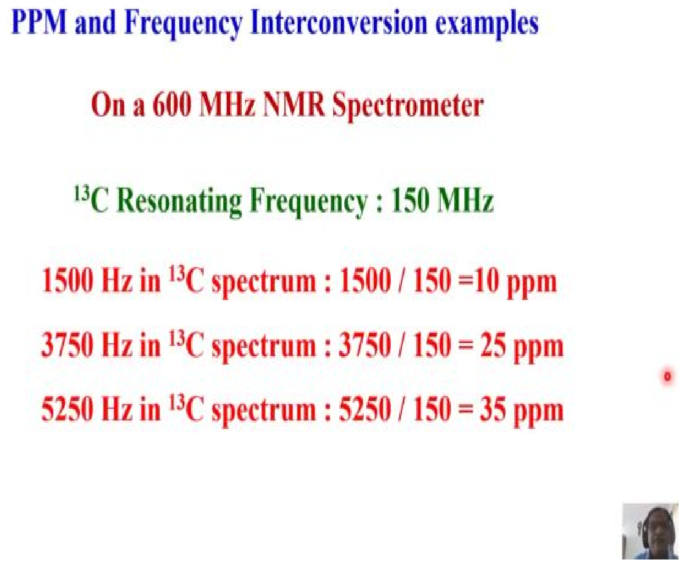

PPM and Frequency Interconversion examples

On a 600 MHz NMR Spectrometer

^{13}C Resonating Frequency : 150 MHz

1500 Hz in ^{13}C spectrum : 1500 / 150 =10 ppm

3750 Hz in ^{13}C spectrum : 3750 / 150 = 25 ppm

5250 Hz in ^{13}C spectrum : 5250 / 150 = 35 ppm

Now, in same way you convert it back, I have 1500 hertz, divide by 150, because in the 600 megahertz, 150 is its resonating frequency, so it is10 ppm. Take 5250 divided by 150, you get 35 ppm. So, ppm to frequency I have given number of examples, ppm to frequency conversion, frequency to ppm conversion. please remember these things are very, very important for understanding.

So what I am going to do is I will stop for the day I told you something about or we were discussing a lot about chemical shifts. Today we discussed about measurement of the chemical shifts in ppm, ppm to frequency conversion, so many references that we use for different nuclei, and what is a ppm everything, we understood. I guess I am taking all of you with me. Hope you all are with me and you are catching up with what I am telling. Please do not forget these are very important points. I am stressing again and again, because these are all fundamentals and specially, when I am doing this course for chemists you should not make mistakes, because you use this NMR spectrum almost every day in your research, so you should understand this concept. We will stop here. We will come back and continue later.