INDIAN INSTITUTE OF TECHNOLOGY BOMBAY

IIT BOMBAY

NATIONAL PROGRAMME ON TECHNOLOGY ENHANCED LEARNING (NPTEL)

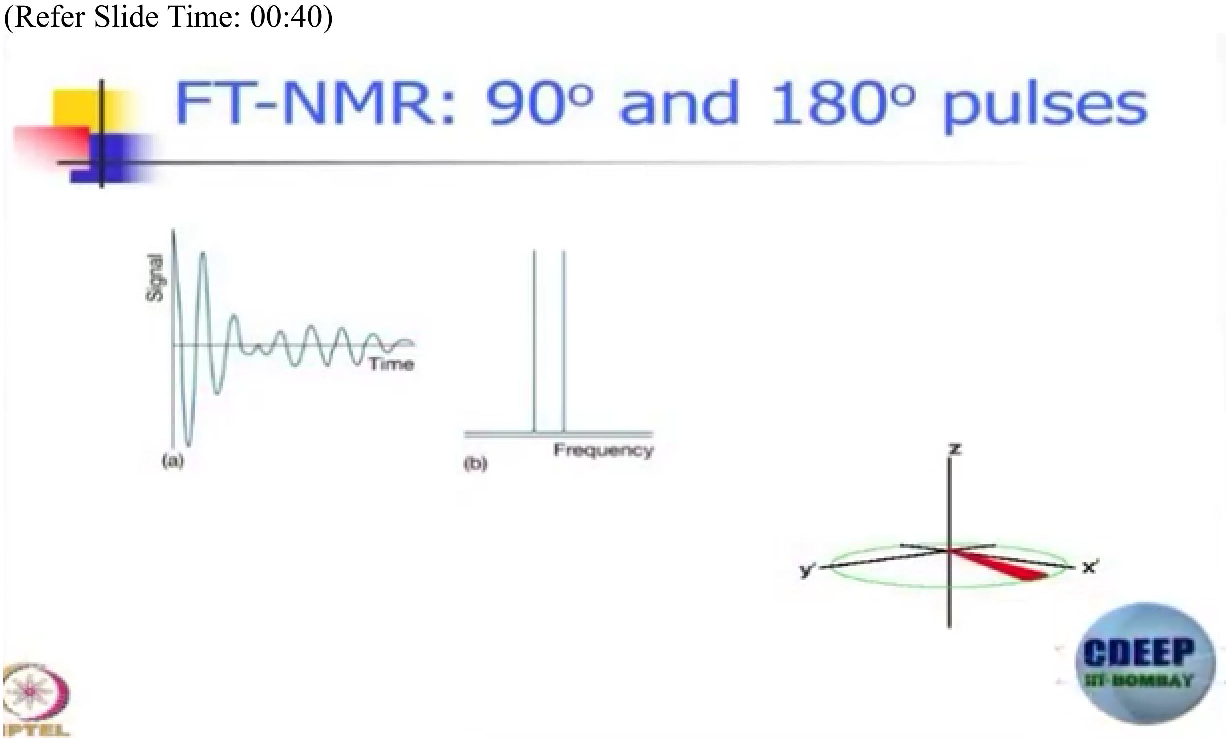
CDEEP IIT BOMBAY

MOLECULAR SPECTROSCOPY: A PHYSICAL CHEMIST'S PERSPECTIVE

PROF. ANINDYA DATTA
DEPARTMENT OF CHEMISTRY, IIT BOMBAY

Lecture no. – 58
FT-NMR: 900 AND 1800 Pulses

Right, we are discussing Fourier transform NMR, and today even though I said this yesterday as well, today we are definitely going to learn what is the meaning of this color patch going around,
(Refer Slide Time: 00:40)

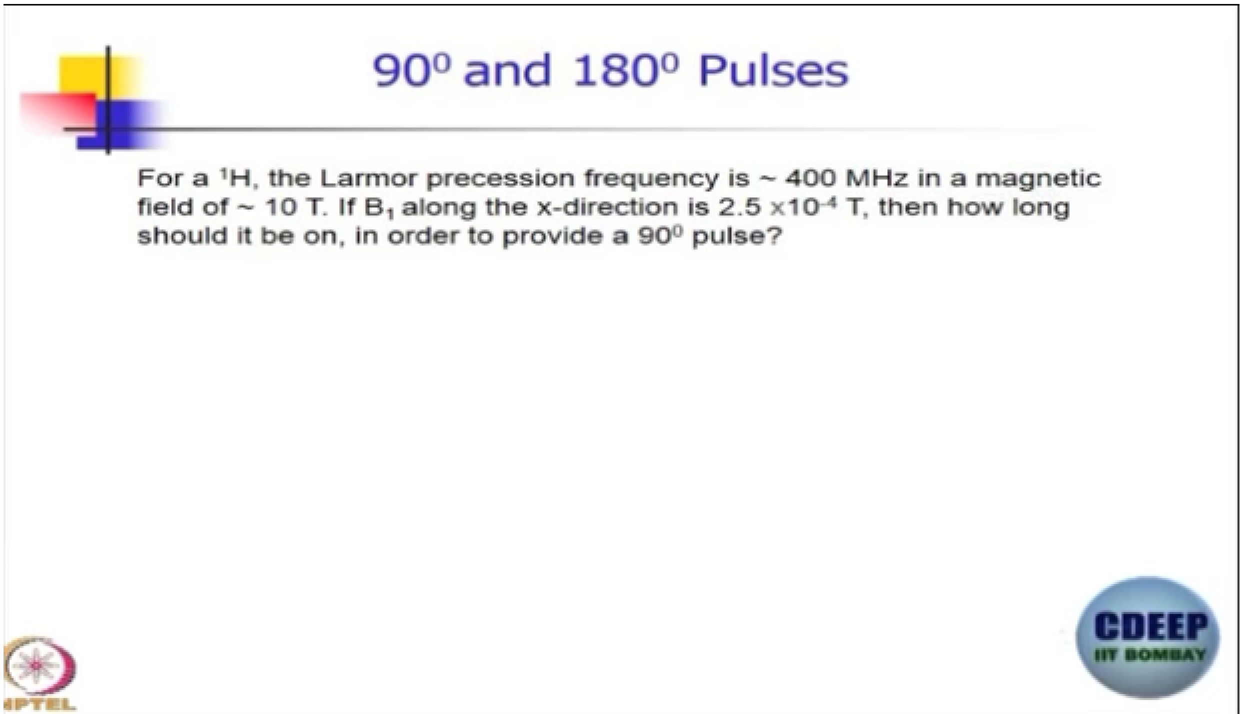


becoming fat becoming thin, we'll learn that today.

This is what we have discussed yesterday, we have discussed how you do NMR measurement by using a 90 degree pulse, so 90 degree pulse is what we discussed in some detail yesterday, so what we said is the way it works is you apply a magnetic field, the moment you apply a magnetic field there is a difference in energies of alpha and beta spin and due to this difference in energies there is a small but perceivable excess of population in the lower energy alpha spin state.

Since that is the case so what we have is we have up spins and we have down spins, number of nucleon up spin is a little more than the number of nucleon down spin, so if you take the vector sum you have the resultant pointing upwards in the same direction as the applied magnetic field, alright that result in vector is your bulk magnetization M0, and we said that in FT NMR what we do is we keep the radiofrequency coil and the detector coil at 90 degrees and that is also at 90, those are also at 90 degrees to the direction of the field so the applied magnetic field, the radio frequency coil and the detector coil are along the three Cartesian access you can think like that, right, great.

So then we said after facing the sample in the magnetic field this is a situation, then we turn on the radio frequency and we denote the magnetic field associated with the radio frequency as B1, so when B1 is turned on we said that this M0 is perpendicular to the direction of B1 so it should start precessing, and in fact as we discussed toward the end of the class it doesn't just precess about the B1 vector, it also has to process about the B0 vector, so this is the one normal mode or circular motion, this is another normal mode, so resultant motion would be something like this. To account for that we have to use a rotating frame of reference which is achieved by using circularly polarized radio frequency light, okay, that being said what you do next is that after a while you turn off the turn B1 off, when I say after a while I mean after the time that is required to turn this bulk magnetization vector through 90 degrees, okay, you told me yesterday that time period is the time required for this bulk magnetization to do one full circle,
(Refer Slide Time: 09:30)



so if I know the time period which is something you can figure out very easily from the frequency of precession then it is not going to be difficult for me to figure out the time that is required for M0 to go through 90 degrees and that's a calculation we'll do shortly.

So after that time turn B1 off, when you do that, now bulk magnetization vector M0 is in the XY plane, since it's an XY plane you can see it in the detector coil which is also along the way we have put it Y axis, Y axis or XZ, X axis sorry X axis, the radio frequency coil is along Y axis, the detector coil is along X axis that's how we've drawn it, and as we discussed when M0 is in XY plane, B0 is still there so M0 will start precessing in the XY plane moreover B0 will try to re-orientated along itself, so the net result in motion will be something like this aspiralinemotion which will eventually result in M0 getting aligned with the direction of the applied magnetic field, right. So this precessional motion as seen by the detector would be a damped oscillation.

If there is a single frequency then it would be a monochromatic wave multiplied by that exponential decay, if you have more than one frequencies which is the case for any kind of molecule that you take then you have an interferogram multiplied by the exponential decay.

We have discussed interferograms at the beginning of the course, we get a interferogram like that, the only difference is now you also get a damped oscillation, interferogram that is really a damped oscillation, so interferogram multiplied by an exponential decay, okay, this is called a free induction decay, and when you do Fourier transform of this free induction then you get the spectra that we actually see, so when we get NMR data out of the machine what we get is this, this is what we understand, but that is not what the machine produces first of all, this is what the machine produces, those of you who are familiar with this computer programming would know that computer programming languages are at two levels right, one is machine language and the other is higher level language like basic or C++ or whatever, that is a language that we understand, the machine understands only 0 and 1, so we always need a compiler or what is it called or basic is not a compiler for Fortran its compiler, for basic what is it called? Yes, interpreter, I forgot that word, in my mind I was thinking translator, translator, interpreter means the same, so this is an interpreter that changes what you have written in the higher level language to machine language something similar happens here, the data is actually produce in time domain but they're just looking time domain it's not so easy for us to figure out which frequencies are there, so after Fourier transformation we get the frequency domain data that we understand.

Is there any question up to this? Do we have any question up to this, than we will answer that and then go ahead. Yes, why decreases? Yes, because so this is M0, right, initially this is how it was along the magnetic field, I've applied B1 so it has turned by 90 degrees and it has come in XY plane, this is where your detector is, so what does the detector see? It sees a large negative signal the way I have put it, then now what we do is that we turn off B0, B0 is not there, but you still have the magnetic field of the, well magnet, right or the machine B0, so two things happened, first is that M0 wants to precess about B0, if this is the only thing that happened and for the sake of simplicity let us say it rotates at one particular frequency then in this detector the signal that you'd get would be an oscillation like this, but that is not the only thing that happens.

See this magnetic field is there, it also tries to re-orientate M0 back and aligned it perfectly with itself, so this is one kind of motion, this is another kind of motion, overall motion is something like this, that's why we get a decay in the, when it's like this the component of the signal along this detector is large, when it is like this component is 0, so that goes from here to here that is your decay.

Any other question? Any other question, yeah, how do we get radio frequency when we apply B1? We actually turn on the radio frequency, radio frequency is an electromagnetic field, right, it has an electric field and a magnetic field, B1 is the magnetic field associated with that radio frequency, any other question? Okay, can we go ahead, okay, so first now you have to do a little bit of work, what is the 90 degree pulse? I have written 90 or 180 but I think I've removed the 180 problem, this is my question, for proton Larmor precession frequency is about 400 megahertz in a magnetic field of about 10 tesla, if you remember what we discussed yesterday, it is not exactly 10 tesla it's 9 point something, and it's not exactly 400 megahertz, it's 398 or something like that, but we can go with this kind of approximation.

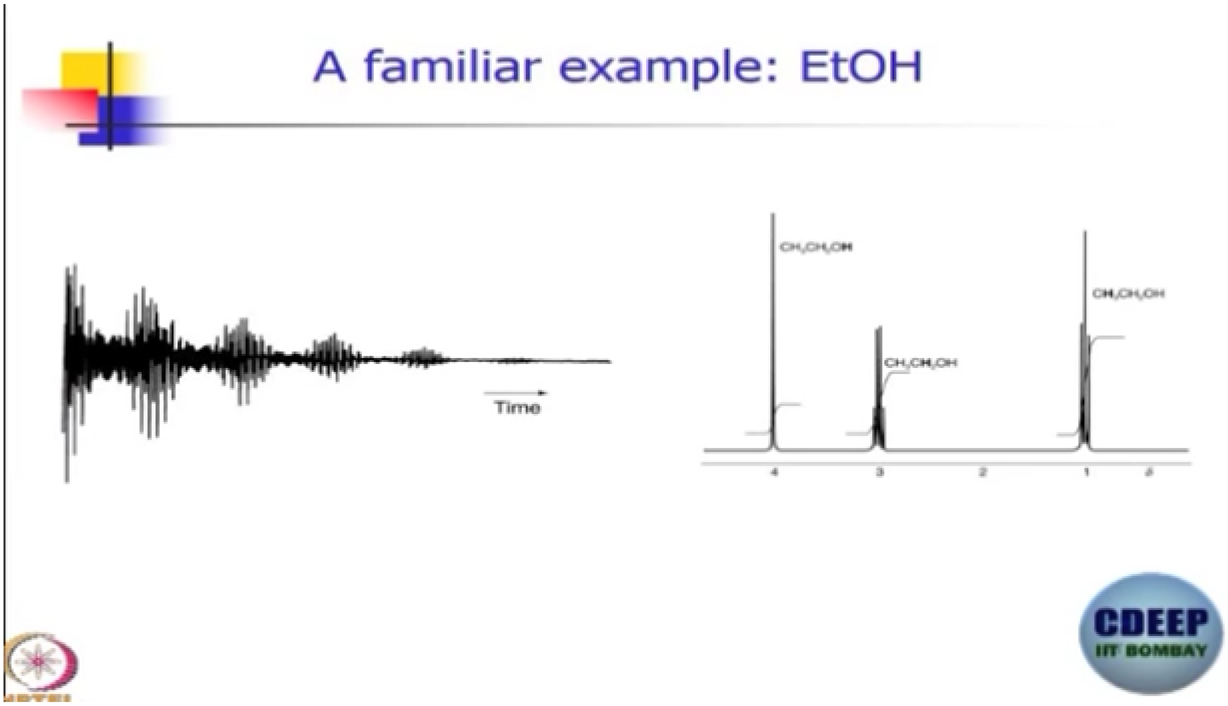
So what I am asking is B1 along X direction is 2.5 x 10 to the power -4 tesla? How long does it take to provide a 90 degree pulse? How will you go about doing it? We know that this precession frequency is proportional to the magnetic field, right, so this precession frequency is 400 megahertz for a magnetic field of 10 tesla, 10 tesla 400 megahertz, so for 2.5 x 10 to the power -4 tesla, what is the frequency? Simple unitary method calculation, tell me what is it? What is the frequency for Larmor frequency for 2.5 x 10 to the power -4 tesla? Simple unitary method calculation right Khader? 10 tesla corresponds to 400 megahertz, 2.5 x 10 to the power -4 tesla corresponds to, yes say that again, 10 to the power -2 and nothing multiplied by it? No, megahertz is okay, so that you have to say right? You only gave me the order of magnitude, now that is the frequency. So if that is the frequency, what is the time period inverse of frequency? What is the time period tell me now? You've found out the frequency by unitary method, what is the time period? Yeah, 200? Pi? No, where did pi come from? Time period is time for one circular motion, so pi should not be there, time period, who will tell me the time period? 10 to the power, -4 or -2? 10 to the power -4 is a time period, now tell me 10 to the power -4 what, what is the unit? Second, so it takes 10 to the power -4 seconds for one complete rotation, right 360 degrees.

How much time does it take to rotate it by 90 degrees? That divided by 4, when you do that you get 25 microsecond, so 25 microsecond is a time for which this radio frequency should be on in order to turn this bulk magnetization by 90 degrees, okay.

Now if I keep it on for 50 microsecond instead of 25 microsecond what will happen? It'll keep rotating further and it will go to 180 degrees, so if you keep this field on for 25 microsecond then you produce what is called a 90 degree pulse, that's what we have discussed, if you keep it on for double the time you produce what is called 180 degree pulse by which bulk magnetization vector is turned by 180 degrees, that's all. Why we want 180 degree pulse that we will see very soon, but have you understood this part? Okay, everybody okay with this 25 microsecond?

So now see we have talked about femtosecond if you remember, so if you are okay with the fact that we can measure femtoseconds, what is microseconds? It's very easy, so microsecond pulses are very easily achieved by using not very complicated electronics, so this is doable, right.

Now of course we have discussed a lot of theory, but as Max Planck had famously said, what did Max Planck said Hrithik, among other things? Yeah, yeah, what was that? You are right, experimental results are the only truth, everything else is poetry and imagination, not to undermine poetry and imagination, that is what separates human beings from other animals, but if you cannot see an experimental result then you cannot accept it as truth, right, that is why people went to such great trouble to do that lego experiment, right, got particle and we have predicted such a long time ago, but people did that really troubles an experiment because after all experimental results are the only truth, so all these discussion of ours that have we have performed there is no reason why you should believe any of it, unless I show you at least one spectrum, and as we have end it there is only one spectrum that we'll discuss in this course that is B1 of ethanol, right, here it goes.
(Refer Slide Time: 14:58)



So this is, the question you were asking yesterday this is the answer to it, when you have many kinds of frequencies and all, this is the kind of spectrum, time domain spectrum that you get, okay, so you see what we get here, well this is the frequency domain spectrum that we are familiar with, in time domain this is what it looks like, so what happens there if you remember is that, not only is there an exponential decay but since there are several frequencies, they keep getting out of step and falling back in step as time progresses, whenever they get back in step you get an enhancement amplitude increases, whenever they go out of step amplitude becomes 0, that is how you generate the interferogram so this here is the NMR spectrum of ethanol and you can think machine language.

If I just show you this will you be able to understand it? I would not understand, I don't know if you can, I cannot, so for us it is essential that we do a Fourier transform and get this spectrum, but this is what is actually recorded in the machine, so if you go and request the operator to let you be there when data is being recorded, the operator can actually show you the FID in NMR machine, but then it is transform an frequency domain data is produced, alright. So far what we have been able to do is we have been able to complete the first part of the discussion that we wanted to do today, that is understand what 90 degree, 180 degree pulses are, and what the spectrum looks like in time domain.

Next we go on to a discussion of how we can use combinations of this 90 and 180 degree pulses to get some data that goes beyond simply recording the spectrum.

Prof. Sridhar Iyer

NPTEL Principal Investigator
&
Head CDEEP, IIT Bombay

Tushar R. Deshpande
Sr. Project Technical Assistant

Amin B. Shaikh
Sr. Project Technical Assistant

Vijay A. Kedare
Project Technical Assistant

Ravi. D Paswan
Project Attendant

Teaching Assistants

Souradip Das Gupta

Hemen Gogoi

Bharati Sakpal
Project Manager

Bharati Sarang
Project Research Associate

Nisha Thakur
Sr. Project Technical Assistant

Vinayak Raut
Project Assistant