Principles and Applications of NMR spectroscopy
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Module 3
Lecture No 14

So we will continue with today with the spectral analysis. So in the last class we have seen how, what are the parameters required for acquiring data and what are the important points for processing. So will now start with how do we interpret with an NMR spectrum, 1D proton spectrum. How do we analyze that data?

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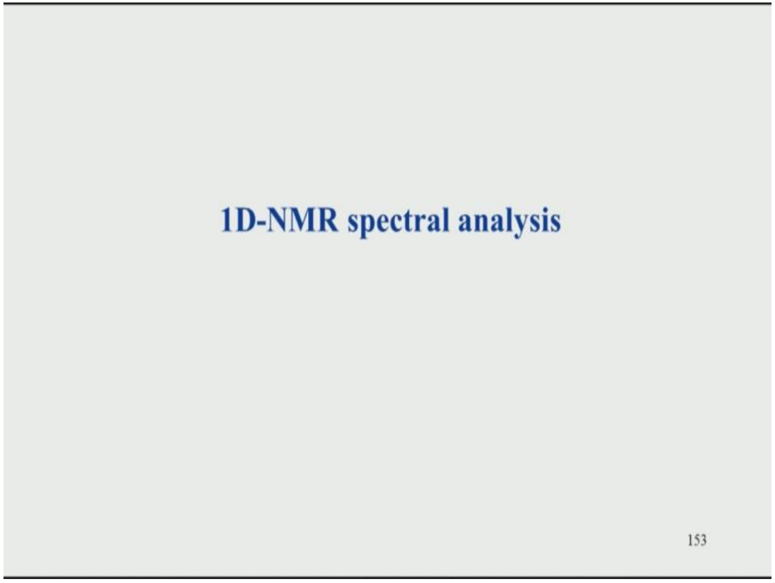
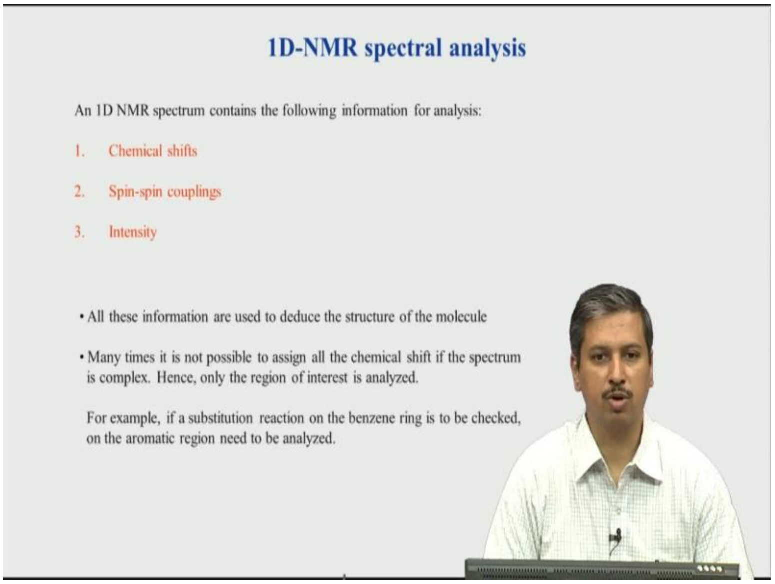


1D-NMR spectral analysis



1D-NMR spectral analysis

An 1D NMR spectrum contains the following information for analysis:

1. Chemical shifts
2. Spin-spin couplings
3. Intensity

- All these information are used to deduce the structure of the molecule
- Many times it is not possible to assign all the chemical shift if the spectrum is complex. Hence, only the region of interest is analyzed.

  For example, if a substitution reaction on the benzene ring is to be checked, on the aromatic region need to be analyzed.

So let us start from 1D proton NMR. So as we see here in a typical 1D spectrum this is what the three parameters mainly you will see. one is called the Chemical shift that is the peak position. You will see what is called Spin - spin coupling. So this is something also we known as J coupling and we saw that it causes split in the peak and there are small multiplets are seen and this has a lot of information about the structure of the molecule.

So therefore it is a very important to also analyze the data in with respect to Spin - spin coupling. then the next parameter which is important for analysis is Intensity. So Intensity is basically the area under the peak. So that again will go through that very briefly. So it is what happens is as written here many times it is not possible to assign all the Chemical shift if the spectrum is complex.

So what we typically do is that is we only look at the region of interest. we will for example says here that if there is substitution reaction in a chemistry. Suppose that there is Benzene ring which gets substituted with some functional group what we do is we just look at the aromatic region because we know that the aromatic region has to undergo a change, if there is a substitution.

So we do not look at the entire NMR spectrum of the molecule. But we only focused on the aromatic. So basically the idea here is that if you have an unknown com. then of course you have to look at the full NMR spectrum and you have to analyze the full data. But if you have only a looking at changes in the spectrum. So if you let us say you have a reaction going on and you know the starting com. and you have the spectrum of that and you have analyzed already the spectrum of the starting com. you are only interested in then looking at the changes happing in the molecule upon substituting or any reaction so in that scenario you do not have to reanalyze the full spectrum, typically what is done is we only look at the region of interest.

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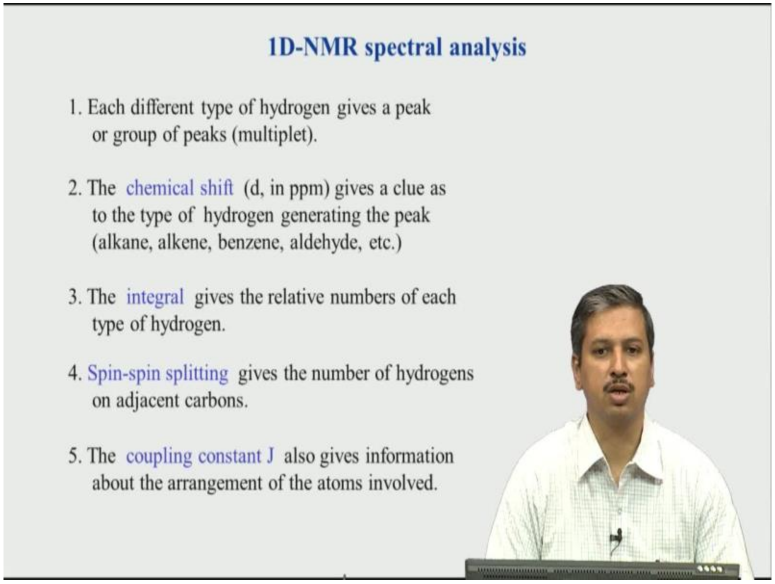

1D-NMR spectral analysis

1. Each different type of hydrogen gives a peak or group of peaks (multiplet).
2. The chemical shift (d, in ppm) gives a clue as to the type of hydrogen generating the peak (alkane, alkene, benzene, aldehyde, etc.)
3. The integral gives the relative numbers of each type of hydrogen.
4. Spin-spin splitting gives the number of hydrogens on adjacent carbons.
5. The coupling constant J also gives information about the arrangement of the atoms involved.

So this is again the repeat of the previous slide, which says what are the different parameters that we have to focus on in NMR spectrum so that we can analyze. So we will go through this as we go on.

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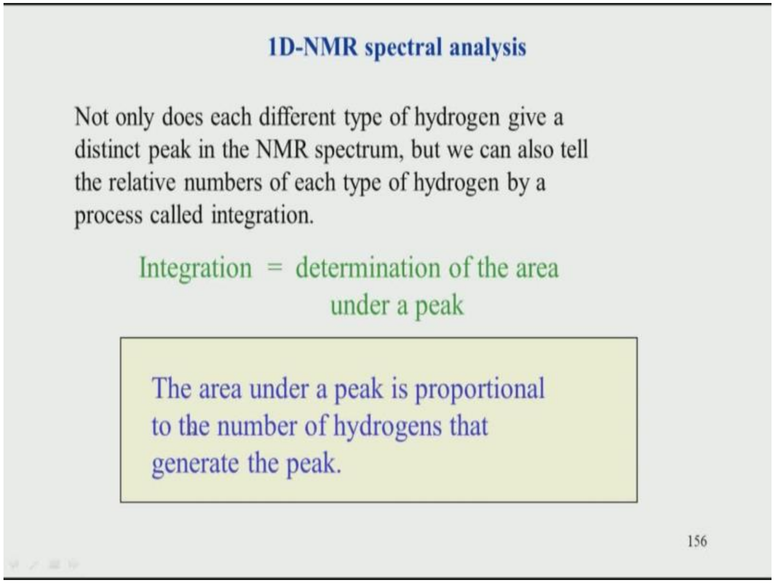

1D-NMR spectral analysis

Not only does each different type of hydrogen give a distinct peak in the NMR spectrum, but we can also tell the relative numbers of each type of hydrogen by a process called integration.

Integration = determination of the area under a peak

The area under a peak is proportional to the number of hydrogens that generate the peak.

So the main thing about the Intensity of a peak what is an Intensity? The Intensity is basically the area. So area which is proportional to the number of hydrogens that generate the peak. So this is a very important point here, is because you know area gives us the total number of protons. And therefore what we do is, we do not actually look at the absolute area, the absolute integration of the peak. But we only look at the relative Intensity.

So for example let us say, you have three hydrogens CH3 CH2 O H. Suppose you take a molecule ethanol. You expect the methyl peaks CH3 to have three times the Intensity as the O H peak, which has only one hydrogen. So the number of hydrogens is is obtained relatively from the number of from the integration value. So the integration value is very helpful for interpretation.

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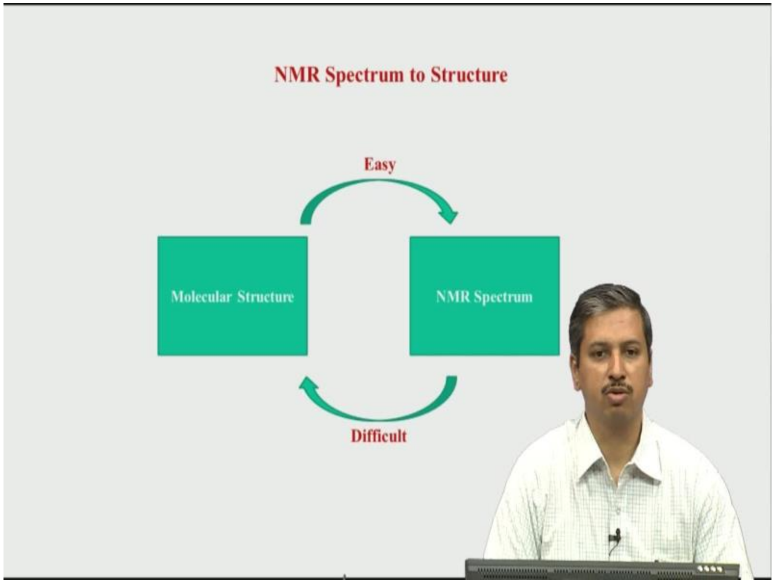

NMR Spectrum to Structure

Easy

Molecular Structure

NMR Spectrum

Difficult

So we will see this now as we go on how these three parameters namely Chemical shift, J J J coupling and structure Intensity is used. Now one thing one has to understand in NMR spectroscopy is that suppose you know the structure of a molecule if you know the molecular structure, you can go from go and generate an NMR spectrum and this is in computer. So if you know, if I know the structure of a molecule, I can generate an NMR spectrum. And similarly if I know the spectrum of a molecule I can get the structure of the molecule.

So this is, this is process is what we typically do all the time going from the right side, there is an NMR spectrum to the left side, which is a molecular structure. But this is not fairly easy. What is easy is this side. Going from the structure to spectrum is fairly easy compared to going from spectrum to structure. So that is the difficult part. And why is this so?

The reason is that is when know if you know the structure of a molecule, you know the chemical composition, you know the various chemical environment around ethyl hydrogen so you can actually compute, calculate the electron densities around every each and every hydrogen. Because you know the structure exactly so there are a lot of software available these days. Which can generate the Chemical shift because Chemical shift remember comes mainly because of the electron density.

So the electron density around a hydrogen atom determines the Chemical shift, the shielding factor and the shielding factor can we be very easily calculated if you know the structure. So generating NMR spectrum means calculating or figuring or predicting a spectrum knowing the structure is very straight forward. But this reverse the inverse approach is very complicated.

So in some cases of course very easy to do that. So that is where the examples which we will take today and and relating the next few lectures the spectrum we will analyze is very simple molecules. So there in such situation is very straight forward. But if you want to go back from structure to spectrum to a structure for a very complicated molecule, such as bio molecules like peptides, proteins it is really a very complicated task.

So it take years of experience given as spectrum to have to get the structure because a lot of manual work involved as well as a software computational methods involved. So our focus will be basically in this part of the course is to look at simple 1D mole, small simple molecule with 1D spectrum and that is mainly proton spectrum in the next few class. But we can of course, we will also include carbon spectrum as we go to the next part.

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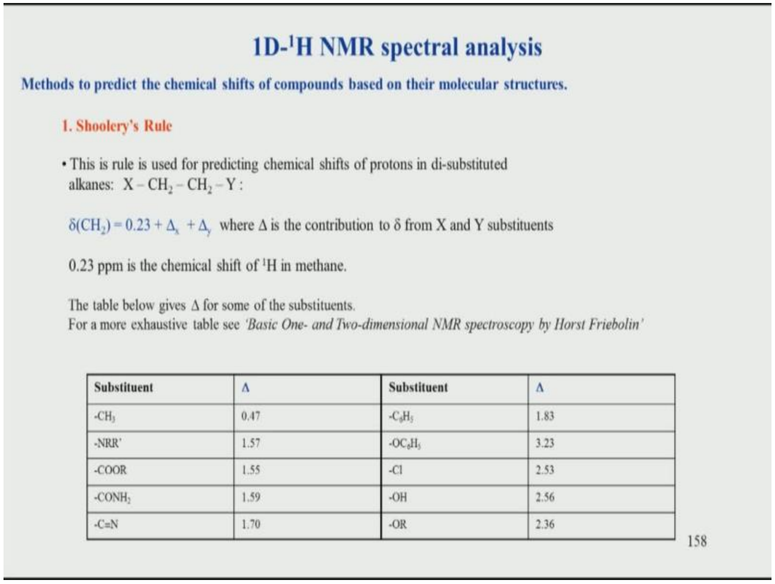

1D-^{1}H NMR spectral analysis

Methods to predict the chemical shifts of compounds based on their molecular structures.

1. Shoolery's Rule

- This is rule is used for predicting chemical shifts of protons in di-substituted alkanes: $X-CH_2-CH_2-Y$:

$\delta(CH_2) = 0.23 + \Delta_x + \Delta_y$ where Δ is the contribution to δ from X and Y substituents

0.23 ppm is the chemical shift of ^{1}H in methane.

The table below gives Δ for some of the substituents.
For a more exhaustive table see *'Basic One- and Two-dimensional NMR spectroscopy by Horst Friebolin'*

Substituent	Δ	Substituent	Δ
$-CH_3$	0.47	$-C_6H_5$	1.83
-NRR'	1.57	$-OC_6H_5$	3.23
-COOR	1.55	-Cl	2.53
$-CONH_2$	1.59	-OH	2.56
$-C\equiv N$	1.70	-OR	2.36

So let us look at what determines the Chemical shifts of a molecules. So there are few rules. Of course this is not, this is not going to be exhaustive list of all the rules which you have there is a very book called by Friebolin 1D and 2 dimensional NMR from where this content has been taken. If you go through that book, you will see many more rules of predicting Chemical shifts.

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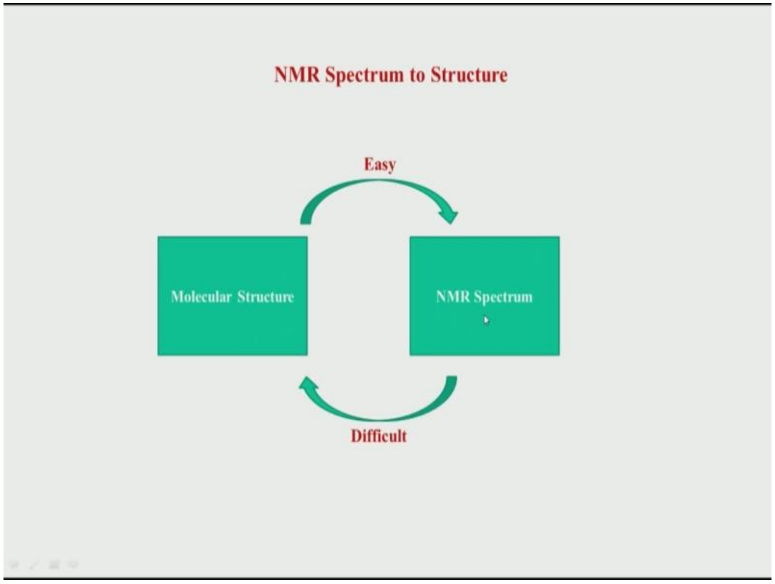

NMR Spectrum to Structure

Easy

Molecular Structure

NMR Spectrum

Difficult

So we are now looking at now we are basically looking this part. So given a structure, can I predict the Chemical shift value of a proton. So we are now going from this to this. Later on we will go from here to here. So let us see given a structure what are the, how, what are the formulas, what are the ways, we can look at generate, predict the values of Chemical shift.

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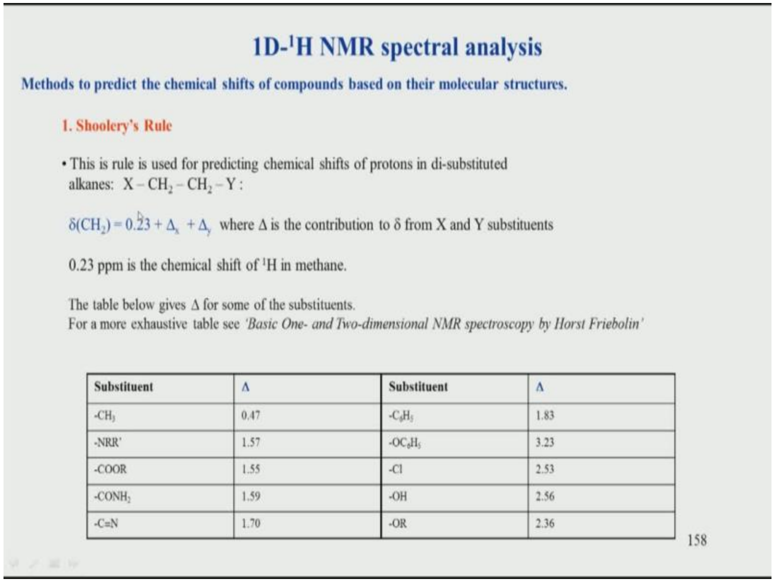

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-C≡N	1.70	-OR	2.36

So NMR spectrum basically means Chemical shift. So when a one of the very first basic rules is Shoolery's rule. here it is applicable to molecules alkanes, which are this type of structures. So you have two CH2s germinal vicinal CH2s and these two CH2s are attached to another functional group, some functional group which may be any any particular functioning group? We do not know that a priory. But let us say this is X and Y. So therefore because this X is not same as this Y we this two hydrogens are not chemically equivalent means this two hydrogens are different from this two hydrogens.

But if X and y are same in that situation we will have a symmetry and such a case then there is a symmetry between the two and then this two will become equivalent. But if X is not equal to Y then you see these two CH2s are not equivalent. So now let us say how do we calculate Chemical shift value of a CH2 group based on the substituents X and Y ok. So this is what is have shown here that there is formula called Shoolery's rule.

You say that you calculate using this approach. You add 0 . 23 PPM to the delta X and delta Y. What are this delta X and delta Y? There is the delta is the contribution to the Chemical shift from X and Y substituents. So this is given in this table. Of course remember this table is again is not exhaustive as written here. You can actually get more exhaustive list from this particular book. So you can see here. For example if I have a substituent CH3 on X and then what I have to do is simply add 0 . 47 to 0 . 23, for this particular depending upon what is X. Similarly, if I have Y another CH3 then I have to basically again add this.

Or if I have some other group, so because we are assuming that X is not as same as Y if I take some other substituent for Y let us say, I take this part carboxylate or ester group or ester moiety then I have to add 1 . 5 ppm to 0 . 23. So that means for a CH2 group here if X is CH3 and Y is C O O R then you will be getting a value for this CH2 like this 0 . 23 + 0 . 47 + 1 . 55. So this is basically how we can calculate for any given functional group for X and Y and then predict the value of CH2. The same thing can be done for this (())(9:47) CH2 as well.

Of course this delta contribution, delta contribution it changes whether X is here or here. For example this is two bonds away. So therefore the delta Y, what is given here delta is basically for one bond contribution. For two bond contribution you have to it will be less and in this book you will get more details on that. But the take home from this slide essentially is there are well defined ways to calculate the Chemical shift of a (mole) proton based on very simple ideas and simple rule provided you know the structure of the molecule.

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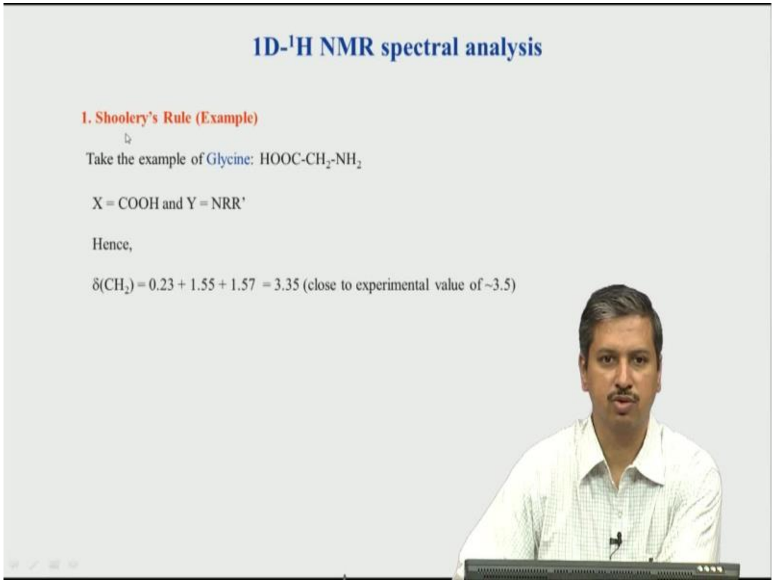

1D-^{1}H NMR spectral analysis

1. Shoolery's Rule (Example)

Take the example of Glycine: $HOOC\text{-}CH_2\text{-}NH_2$

X = COOH and Y = NRR'

Hence,

$\delta(CH_2) = 0.23 + 1.55 + 1.57 = 3.35$ (close to experimental value of ~3.5)

So let us look at some examples of this case. Let us say, we have an amino acid called Glycine. In a Glycine you can say here, the X is COOH and the Y is NRR. So if i want to calculate the Chemical shift of this CH2. Then what I will do, I will use this Shoolery's rule and you add this 0 . 23 and then you add 1 . 55, we saw that for COOH in the previous slide and 1 . 5 for NRR, 1 . 57. So you will get around a 3 . 35 and interestingly turns out then the experimentally, when you actually record a spectrum, 1D proton spectrum of Glycine you will get a value around point around 3 . 5.

So you see it is pretty well very much matching within error little bit of error with the Chemical shift. So can see this, theoretic this is a theoretical prediction. So what we are doing here we have theoretically predicting the value of the Chemical shift based on the rules and that seems to match very well with the. So this is the Empirical formula.

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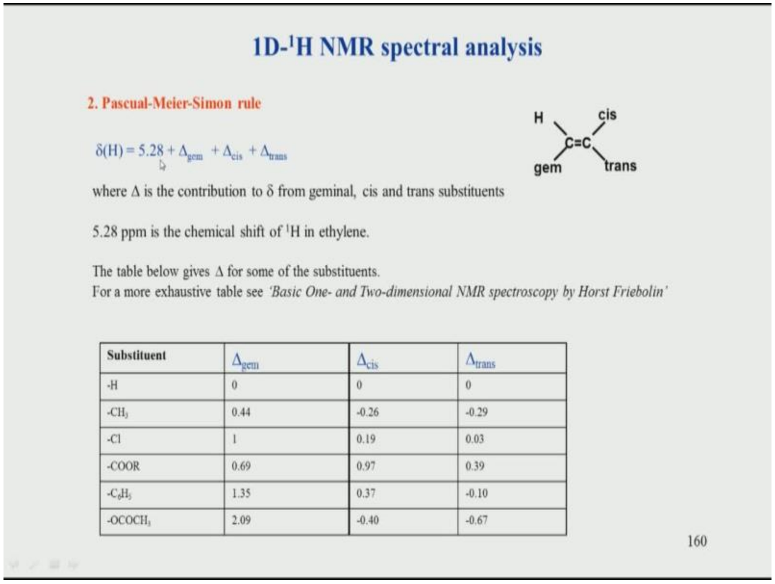

1D-^{1}H NMR spectral analysis

2. Pascual-Meier-Simon rule

$\delta(H) = 5.28 + \Delta_{gem} + \Delta_{cis} + \Delta_{trans}$

where Δ is the contribution to δ from geminal, cis and trans substituents

5.28 ppm is the chemical shift of ^{1}H in ethylene.

The table below gives Δ for some of the substituents.
For a more exhaustive table see *'Basic One- and Two-dimensional NMR spectroscopy by Horst Friebolin'*

Substituent	Δ_{gem}	Δ_{cis}	Δ_{trans}
-H	0	0	0
$-CH_3$	0.44	-0.26	-0.29
-Cl	1	0.19	0.03
-COOR	0.69	0.97	0.39
$-C_6H_5$	1.35	0.37	-0.10
$-OCOCH_3$	2.09	-0.40	-0.67

Now there is another rule called Pascual Meier Simon rule, where you can use again this is now meant for molecules which I have some structures like this ok. And in this particular situation, again if you look this hydrogen atom, you are trying the calculate the Chemical shift of this hydrogen. It depends on what are the substituent present here, here and this geminal position and cis and trans. So you can see how this you calculate.

You take the, you add five points. This is a constant take a five point. All these are derived empirically based on the absorbed spectrum and a large data base, large number of molecules spectrum which were recorded. And then some there it has been calculated. So again this is taken from this book by Horst Friebolin and that book has much many more details subsequent values given. So here, So let us, take this particular case so you have 5.28 + you add the delta geminals.

So depending on what is present in the germinal from this list here, you take this contribution. For example let us say this hydrogen is present in a geminal position here. So in this molecule there is a hydrogen nothing is added to this. That means it is the 5 . 28 remains as such. So it does does not contribute to the Chemical shift of this hydrogen I mean to this formula. And then you have a cis here, delta cis. That is it is the cis position.

Again hydrogen does not contribute and similarly transfer. Basically if you have all this substituent as hydrogen. There is no substituent this all are hydrogen, this is basically ethylene and if you recollect ethylene molecule we saw the Chemical shift that was around 0 . 5, 0 . 23 or

5 . 28 which is shown here ok. So that is the pure ethylene. But now you start substituting different functional groups then you have to use this table to calculate the contribution each of this groups to the total Chemical shift value.

So let us take for example here methyl. So if I have methyl here, methyl here and methyl here. So suppose I have all three positions methyl all have to do is simply add 0 . 44 + (- 0 . 26) - 0 . 29 roughly they will cancel out. We will have a little bit of negative and this will be subtracted. That negative will be subtracted from 5 . 28. So we based on this approach you can now extend this to different functional groups.

You can take all combination, you can have chorine atom at this positions and you can consider hydrogen here, methyl here and all possible combinations.

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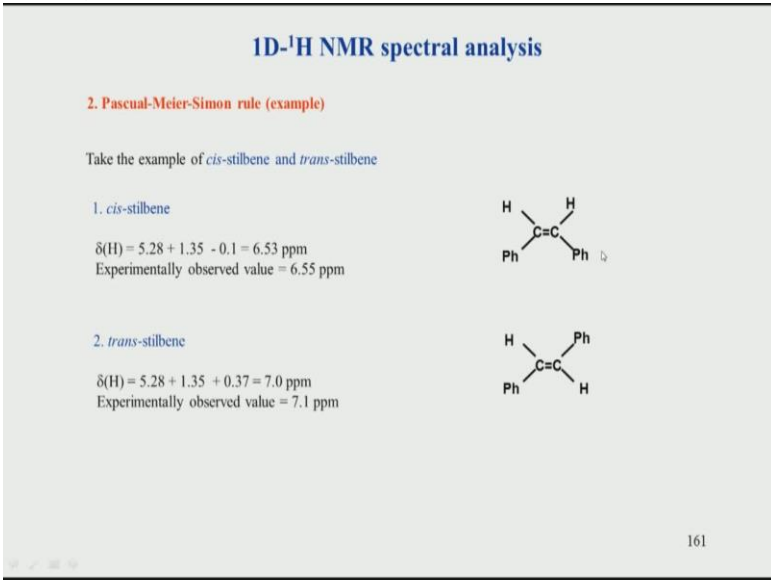


1D-^{1}H NMR spectral analysis

2. Pascual-Meier-Simon rule (example)

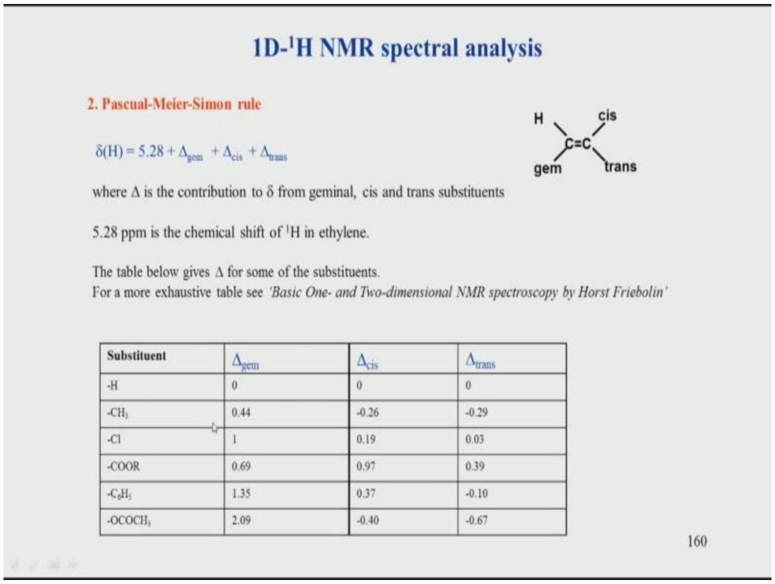
Take the example of *cis*-stilbene and *trans*-stilbene

1. *cis*-stilbene

$\delta(H) = 5.28 + 1.35 - 0.1 = 6.53$ ppm
Experimentally observed value = 6.55 ppm

2. *trans*-stilbene

$\delta(H) = 5.28 + 1.35 + 0.37 = 7.0$ ppm
Experimentally observed value = 7.1 ppm



1D-^{1}H NMR spectral analysis

2. Pascual-Meier-Simon rule

$\delta(H) = 5.28 + \Delta_{gem} + \Delta_{cis} + \Delta_{trans}$

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So you can see this is a very interesting thing. What this rule says, that all these rules which are we are looking at right now it says that it is a linear additive effect to Chemical shifts. So that is a very interesting thing and that is why as I mentioned that is very easy to go from a structure. If you know the structure to the spectrum I mean that is to calculate chemical the shift, knowing it a vice versa is little complicated. So now let us see here in the example the application of this Pascual Meier Simon rule you can see here that in this particular case there are phenyl substituent, phenyl group, Benzene rings, phenyl group on this cis position geminal position and trans position, whereas hydrogen is here.

So based on this previous slide here. You can see for the phenyl group what is the contributions to be taken into account based on their position. And hydrogen also we know, what is the values to be added. So that is what is shown here. That you will basically get when you add this two contributions, you will get 6 . 53. Because remember hydrogen is zero. So hydrogen is not coming into picture here. So this is 6 . 5 and this will very well matches very nicely with the experimentalyl absorbed value ok. So that is very interesting.

Similarly if you look at trans stilbene, this was cis stilbene. If you look at trans stilbene, now their ph the phenyl group in this cis position that is in germinal. And this hydrogen has come to the trans. So again if you look at this contribution again hydrogen, this hydrogen is not contributing according to the rule. It has no, zero contribution. So we are looking at only at the phenyl ring and based this is all looking at this table here. You can see for phenyl ring, if it is in the cis position, it has to be 0 . 37 and If it has germinal is 1 . 35 and that is what is done here. You add 1 . 35 + 0 . 37 to 5 . 28 you get 7 PPM.

Again matches very nicely with the experimentally observed value. So you see this formula has been, how been generated based on observing the chemical shifts of a large number of molecules and then dissecting out the contributions of each of this functioning group to a given hydrogen.

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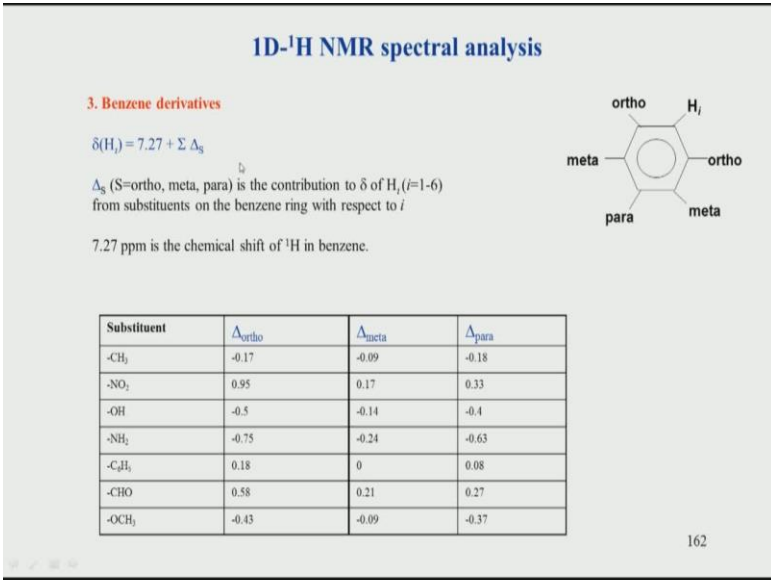

1D-^{1}H NMR spectral analysis

3. Benzene derivatives

$\delta(H_i) = 7.27 + \Sigma \Delta_S$

Δ_S (S=ortho, meta, para) is the contribution to δ of H_i (i=1-6) from substituents on the benzene ring with respect to i

7.27 ppm is the chemical shift of ^{1}H in benzene.

Substituent	Δ_{ortho}	Δ_{meta}	Δ_{para}
$-CH_3$	-0.17	-0.09	-0.18
$-NO_2$	0.95	0.17	0.33
-OH	-0.5	-0.14	-0.4
$-NH_2$	-0.75	-0.24	-0.63
$-C_6H_5$	0.18	0	0.08
-CHO	0.58	0.21	0.27
$-OCH_3$	-0.43	-0.09	-0.37

So we go to the next tool, which is applicable to derivatives of Benzene. Remember in a phenyl ring, in a aromatic ring you have substituent at different positions. You can have it ortho, meta and para and each of these groups contributing a different manner. So this again if you recollect we saw this in the Mesomeric effect or Inductive effect where we see that depending on where the substituent are there could be a resonance structure and shift of the electron, the charges around this different carbon atom.

And based on that the para, meta, ortho play a different role in different roles in contributing to the Chemical shift. So therefore here we also can see that for a given substituent in this column, its contribution when it is present in different position has been written here, shown here and they are all different values. So you see the same CH3 group, whether it is in the ortho position or meta or para it has slightly different contributions to the total Chemical shift.

Same thing with the OH it is depending on very differently so if it is in meta, it is contribution is very much different from ortho and para. Typically ortho and para, ortho and para are contribute to a similar order. Whereas meta you will see in many cases are widely different. So this is typically the trend we see. That the ortho and meta, ortho and para positions contribute to this positions this hydrogen atom in a similar to the similar order, whereas meta has a completely different contribution.

So we can just simply add up all these values depending on where it is present and we can calculate. So 7 . 27 is basically the standard here when all the substituents there is no substituent and all are hydrogens, protons. So the full all are protons basically it becomes a pure Benzene ring. And the Benzene ring, Benzene has Chemical shift of this. So that is why when you have hydrogens, you have to make it zero.

There is the contribution of hydrogen here, here, here to this Chemical shift. It will be already taken into account into this value and that will 7 . 27.

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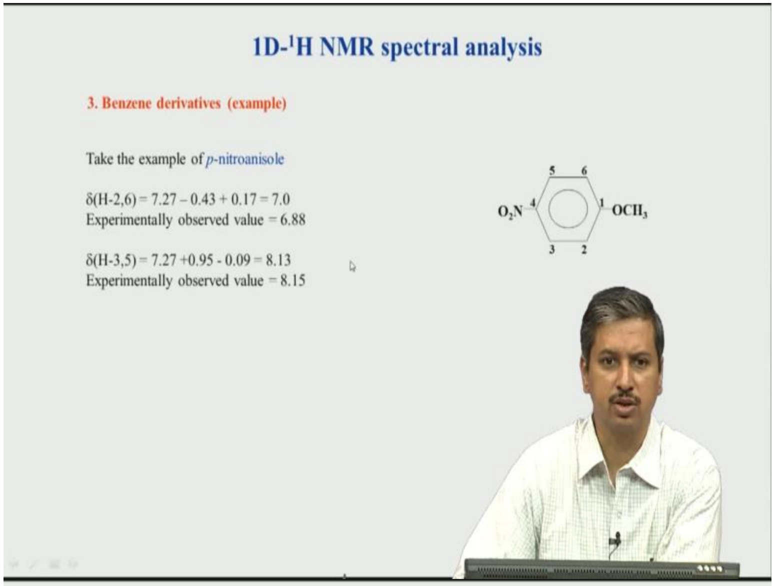


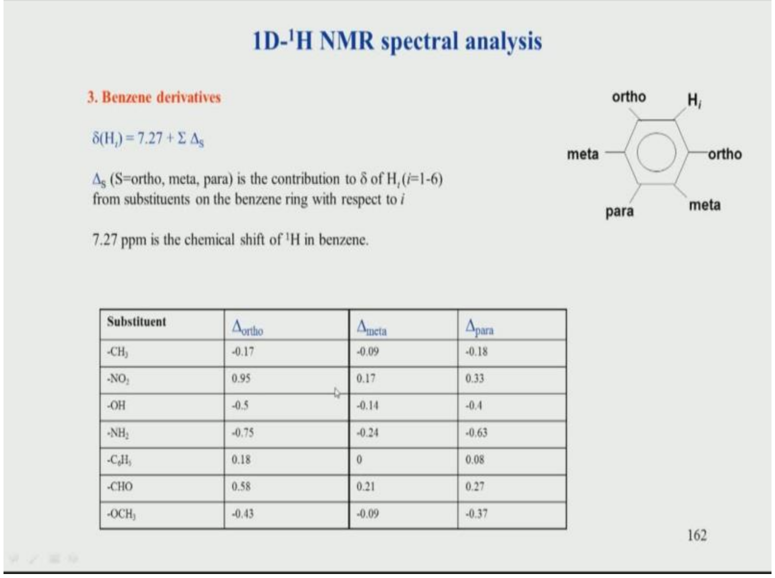
1D-^{1}H NMR spectral analysis

3. Benzene derivatives (example)

Take the example of *p*-nitroanisole

δ(H-2,6) = 7.27 – 0.43 + 0.17 = 7.0
Experimentally observed value = 6.88

δ(H-3,5) = 7.27 +0.95 - 0.09 = 8.13
Experimentally observed value = 8.15



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Δ_S (S=ortho, meta, para) is the contribution to δ of H_i (i=1-6) from substituents on the benzene ring with respect to *i*

7.27 ppm is the chemical shift of ^{1}H in benzene.

Substituent	Δ_{ortho}	Δ_{meta}	Δ_{para}
$-CH_3$	-0.17	-0.09	-0.18
$-NO_2$	0.95	0.17	0.33
-OH	-0.5	-0.14	-0.4
$-NH_2$	-0.75	-0.24	-0.63
$-C_6H_5$	0.18	0	0.08
-CHO	0.58	0.21	0.27
$-OCH_3$	-0.43	-0.09	-0.37

So let us see some calculation, examples of this case. So you can see this is para nitroanisole. Here you can see this now nitro group is in the para position. And we are trying to now calculate the Chemical shift of these hydrogens. So we are looking at this hydrogens, this hydrogen and these two hydrogens. So you can see for calculating for number two now two as when we look at hydrogen in position two, now we are looking at the contribution of O CH3.

Which is ortho to two and it is meta for NO2 ok. So similarly it is same for six. When it look at six, they are these two are now chemically equivalent. So we consider them together, their one Chemical shift because of a symmetry axis here. So these two are equivalent, similarly three and five are equivalent. So when two and six we are considering we have to look at the contribution of the book into meta position to this six Chemical shift here of six. So we can go back to the list here.

We can see in the meta position, if cis if it is ortho position, if there is CH3 it has this value of - 0 . 17 and nitro in the meta position has this value. So that is what is shown is the OCH3. So if you go back the OCH3 is shown here. So in the ortho position you have to take into account this number here - 0 . 43. And for nitro in the meta position it is 0 . 17 and that is what is done here - 0 . 43 + 0 . 17 so 7 . 27 was a base value. So you get 7, 7 . 0 which is again very close to what you expect up experimentally.

Now if you look at these two hydrogens three and five. In a similar manner we can now calculate the contributions of OCH3, which is now meta two five. And meta two two or meta two three and nitro group is now ortho two five and ortho two three. And therefore you have to look into the table in the previous slide. And you will get the values like this, say if you add all of them. You get 8 . 13 and again very and again very very close to the experimentally.

So typically of course the rule of thumb in NMR is generally 0 . 02, 0 . 03 in proton values are within error. This you can probably consider it as slightly away from the experimental value is about 0 . 12 ppm. But remember in the proton 0 . 02 is really close. You can’t get better than this, because error value in measuring based on line width and So on and again depends on the spectrometer we use. And typically 0 . 2 ,0 . 3 would be the best resolution and good resolution which you can expect to get in an NMR experiment, spectrometer.

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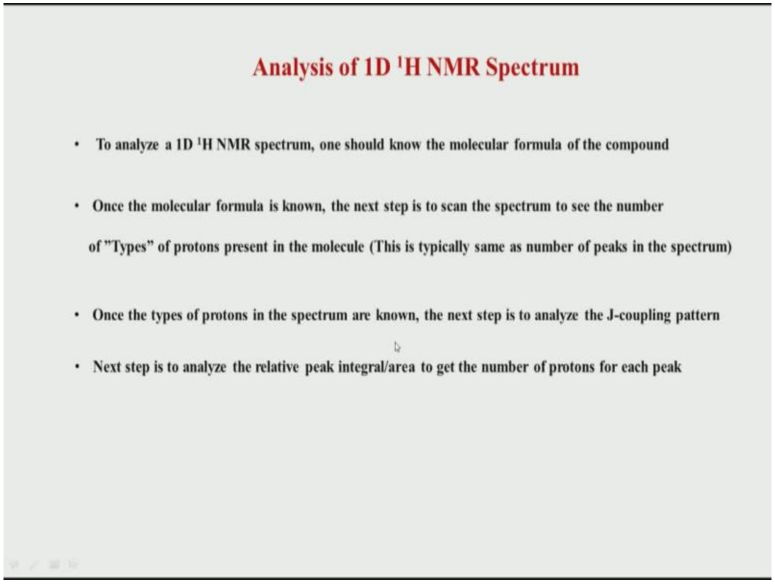

Analysis of 1D ^{1}H NMR Spectrum

- To analyze a 1D ^{1}H NMR spectrum, one should know the molecular formula of the compound
- Once the molecular formula is known, the next step is to scan the spectrum to see the number of "Types" of protons present in the molecule (This is typically same as number of peaks in the spectrum)
- Once the types of protons in the spectrum are known, the next step is to analyze the J-coupling pattern
- Next step is to analyze the relative peak integral/area to get the number of protons for each peak

So now that is basically how we look at the analysis of 1D NMR spectrum. We as I said, if you want to look a so what we saw in the previous slide was basically all the different formula, rules we only showed about three rules. There are as you say the N number of rules which we will not be able to cover in details each and every in this course. Therefore I would strongly recommend to go through this book by Horst Friebolin and many other books have this formulas and this is a good data base, is like a reference formula you do not have to memories them. But one have one can keep in there, in you are hand book as a reference.

So whenever you want to and basically all the softwares, whatever we have this day they implement all these rules. So when we come to the later part I will I will give a list of software and which be nowadays are very popularly used. Many of them are freely available on the internet, can be downloaded and used. And all this software basically are implementing this type of formulas.

So now we will now come to the second part, where we given a spectrum can we predict the structure. So this is a reverse approach. So in the approach was given a structure already given if I know the structure can I predict the Chemical shift value and that is very as I said. but if you know the structure, spectrum and you want to get to the structure that is not straight forward. Reason being that you do not have any clue about what functional groups are present.

All you will have is a molecular formula. This is what you say the first thing you should know if you want to go from a spectrum, spectrum to structure you should be very well aware of about the molecular formula. Without molecular formula it is very difficult to figure out what the structure could be. So one should have at least a basic idea or accurate idea about the molecular formula. That means what are the C H, how many carbons, how many oxygenss, how many nitrogens are present.

You may not be knowing whether there is ester group or in a carboxylate group or aldehyde group or in alcohol So on. That is fine and that is not required and that will use based on our known ideas. But at least one should know accurately how many carbons are there, how many hydrogens are present in your molecule and how many this one, how many nitrogens are there. So we will look at all these things now. So now one of the once the molecule formula is known the next step is to scan the spectrum and see how many types of protons you are able to see in the spectrum.

So these are of course all these rules will go through it again in a real example. So the point here is that remember type of proton, what do you mean by proton type? It means that this set of a proton will have the same Chemical shift value. They are chemically equivalent. So let us say the CH3 CH2 OH, if you see in this menthe, ethanol you have CH3 which is one type, CH2 which is another type and O H is the third type. So you see there are three types of proton in this molecule.

That mean CH3 will give you one peak, CH2 will give you another peak, O H will give the third peak. So based on the looking at the number of peaks in the spectrum corresponds to number of types of protons. This is a very typically the second step after you know the chemical formula. This is a second step you have to scan the spectrum or look at inspect the spectrum to look at the number protons in your sample in your molecule.

Then once you know the number of protons what you have to the next start analyzing the J coupling pattern ok. So J coupling is the pattern is very important, because J coupling tells you the nearby number of hydrogen. For example CH2 CH3 O H there is technical ethanol you see that in that CH2 will have a quartet because of the splitting of, because of three protons. Methyl CH3 will have a triplet because of two protons.

And remember all this triplet, quartet and all etcetera coming from the Pascal’s triangle which we saw in the last few previous classes. We will go through that again quickly. So analyzing a J coupling pattern is very important is very next step. So you first you know the number of protons present in you are molecule. Then you look at the J coupling pattern and then once you know this three, once you know this two thing the next step is basically know looking at the integral or area of the peaks to get the number of protons for each peak.

And this is very important because now next thing is once you know the number of the proton types of protons present you need to know, how many protons are present in each type. So let us again take the example of ethanol which is CH3 CH2 OH in that molecule CH3 has three protons, CH2 has two protons and OH is one Proton, So you can see if you look at the integral, you would, you should expect to get integration like three is to relative integration. Remember we are always talking about relative NMR is three is to two is to one ok.

So now relative integration now helps you to know that how many protons are present in each type. And that information is very useful because once unless you know the number of protons in of each type you will never, you will not be able to figure out whether the total number of protons are matching with your molecular formula. So remember the molecular formula gives you the total number of hydrogens in your molecule and that should match with the total relative peakings.

So for example again coming to this three is to two is to one that means I should expect six protons three + two + one. And so in CH3 CH2 O H there are six protons. So you see the number of protons, which I can, which I will calculate from peak integral should match exactly the number of protons available to be in the formula. Otherwise if there is a mismatch then you will not be able to analyse. Because that means there is a missing proton somewhere that will not help you to analyze.

So the missing proton is the only information available is here. Of course many time, this is based, this the whole sequence shown here is only for the hydrogen spectrum. But remember, we can only use the carbon 13 NMR spectrum to also get the information on the type of carbon group here. So the molecular formula has also. So remember we are going to look at only organic com. in the next few slide. So the organic com. is what we are going to analyze not biomolecule as of now.

So in organic com.s the main molecule, atoms are carbon and hydrogen. So carbon spectrum is also an essential but at this stage in the next class we will see that how we can use mainly based on proton spectrum to get from the structure formula molecular spectrums, the spectrum of the molecules to the structure. And from that itself for very simple molecule the hydrogen spectrum is sufficient to do that. But carbon spectrum also is useful when you go to the more complicated molecule. So will see this in the next class, how hydrogens spectrum can be analyzed based on these rules.