One and Two Dimensional NMR Spectroscopy for Chemists
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Lecture - 24
Coupling among Equivalent Spins

Welcome back in the last class, we discussed various things about scalar couplings and we started discussing about signs of the couplings. Remember, I mentioned about the signs of the coupling especially, how to arrive at the sign.

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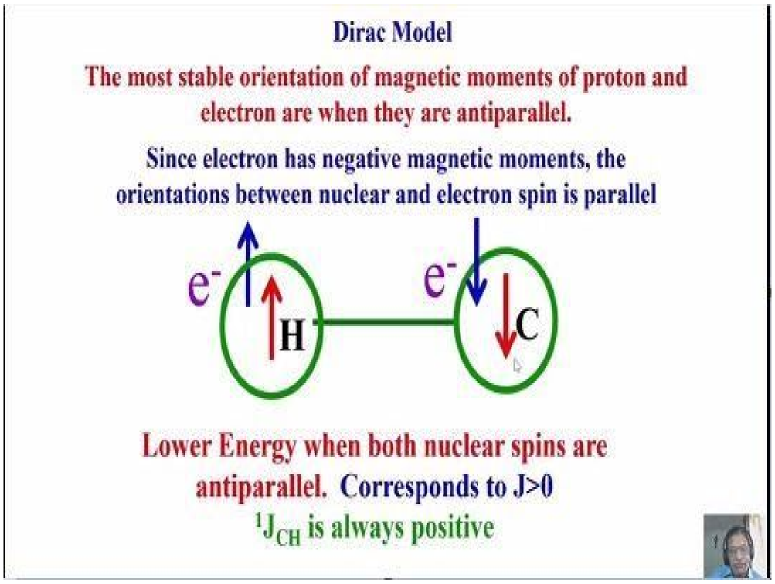

Dirac Model

The most stable orientation of magnetic moments of proton and electron are when they are antiparallel.

Since electron has negative magnetic moments, the orientations between nuclear and electron spin is parallel

Lower Energy when both nuclear spins are antiparallel. Corresponds to $J>0$

$^1J_{CH}$ is always positive

We started looking at first important thing, by a Dirac model. What is the sign for one bond CH coupling, we understood, because it is the orientation of the one of the magnetic moments of one of the nuclei, if you consider of the coupled one, like proton and carbon, if they are chemically bonded, if you see the orientation of proton spin, if it is in the direction parallel to the field, because of this Fermi's contact, Pauli pairing and again Fermi contact, using this Dirac model, this orientation forces the carbon to orient in a direction anti-parallel to it. As a consequence, I said this is lower energy state and stable configuration, and it corresponds to the energy state in such a way the J coupling is greater than 0. That means, 1JCH is always positive.

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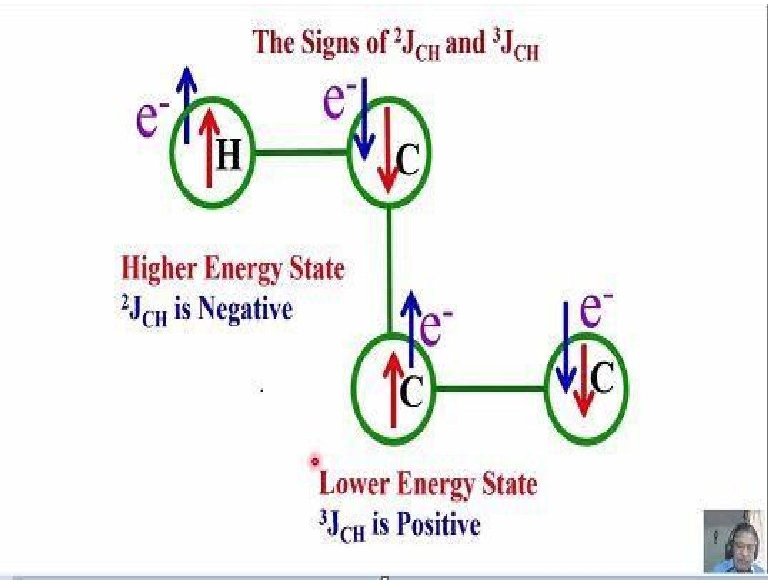
The Signs of $^2J_{CH}$ and $^3J_{CH}$

Higher Energy State
$^2J_{CH}$ is Negative

Lower Energy State
$^3J_{CH}$ is Positive

And we also have worked out 2JCH that is negative, we also worked out 3JCH that is again positive, in a simple model like this. We worked out based on the orientation of the nuclear magnetic moment of one of the protons or one of the nuclei of the CH bond, and then proceeded further from a Fermi contact, Linus Pauling pair, and then again, Fermi, Linus pairing, like that we went through the various bonds, all the 3 bonds and we arrived at the sign of the coupling, and we found out 3JCH is positive, that is fine.

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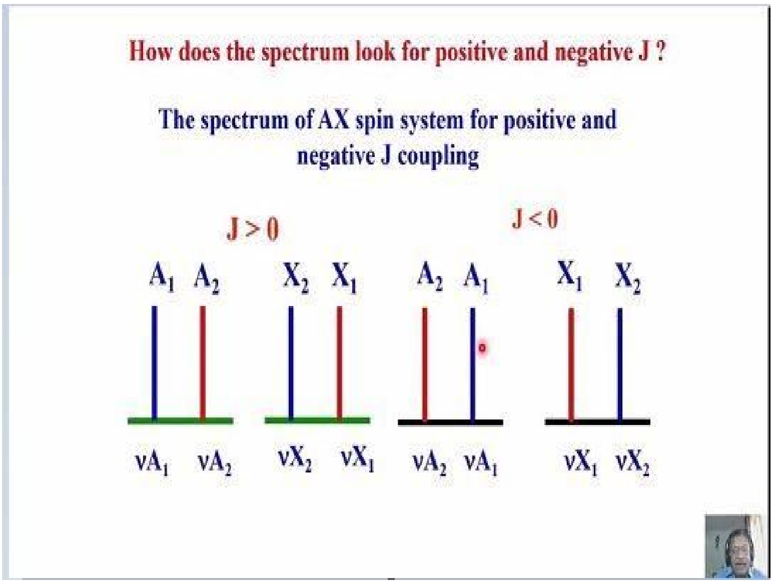
How does the spectrum look for positive and negative J ?

The spectrum of AX spin system for positive and negative J coupling

Now, how does the spectrum look for positive or negative sign of the coupling? As I said CH coupling is positive for 1JCH and 2J CH is negative. Suppose I take a spectrum, in one case let us say, that the sign is positive. In the other case, I will say sign is negative. How does the spectrum look? That let us understand. Now I consider the situation of 2 coupled spins. Maybe it is a CH coupling, carbon and proton, does not matter, we consider a situation. We know one bond carbon proton coupling. We know J is positive for it and if I consider the spectrum, assume a situation both carbon 13 also highly abundant, in the sense it is the labeled system. In which case, I look at the proton, I get the 2 peaks, I look at the carbon, I get 2 peaks. It is an AX spin system, 2 lines for proton and 2 lines for carbon. Now I am plotting one next to each other. This is for the A spin proton, this is X spin carbon 13.

From our energy level diagram and all the splitting pattern we understood when 2 protons or 2 nuclei are coupled homo or heteronuclear, does not matter, from the energy level diagram we observed that we get 2 peaks for A and 2 peaks for X of equal intensity. We also worked out based on the transitions, how the transitions take place within 2 energy states, which spin is flipping, we also found out which transitions pertains to A spin, which transition pertains to X spin. Both we understood, That is how we identified 2 A transitions and 2 X transitions.

I hope you remember the energy level diagram, with which you worked out transitions for both A and X. Let us say, this is the pattern I am going to get, for J greater than 0. Most important you have to monitor A1, A2, X2, X1. These are the numbering I have given for transitions A and transitions X. That we know, the transitions we have already worked out. Consider the situation now, J is less than 0. That is J is negative. What is the difference you are seeing here except, because I have colored for to make you understand, you will not find any difference because in the real spectrum.

When you record 1D spectrum, there is no coloring of the transitions. Just to make you people understand, I made one transition of A, one transition of X has different color. For J positive, J greater than 0. Now J is greater than 0, if you look at this spectrum, you see A2 has come here A1 is moved here. You understand, X1 has come here and X2 is moved here. So, you understand A1 and A2 got interchanged here. And X1 and X2 got interchanged here, which is fantastic.

But you if I do not color A, and if I do not tell you anything, you will not know which transition is which, because you do not go and find out by the energy level diagram every time. Simply I will give you a spectrum with J greater than 0. I will give you another spectrum with J less than 0. And I will give you independently both of them. You will not find the difference. You will find everything is overlapping the way it is. Only thing is internally lines like this would have interchange with the change of sign.

Remember what happens, look at this, these 2 lines are like this, and they get reversed. That is all. The transitions get its interchange between the coupled spins, but you will not find any change in the appearance of the spectrum apart from that. So, as a consequence, the spectrum is invariant with respect to the change of sign, if the coupling is either positive or negative from the one dimensional spectrum it is not possible for you to find out.

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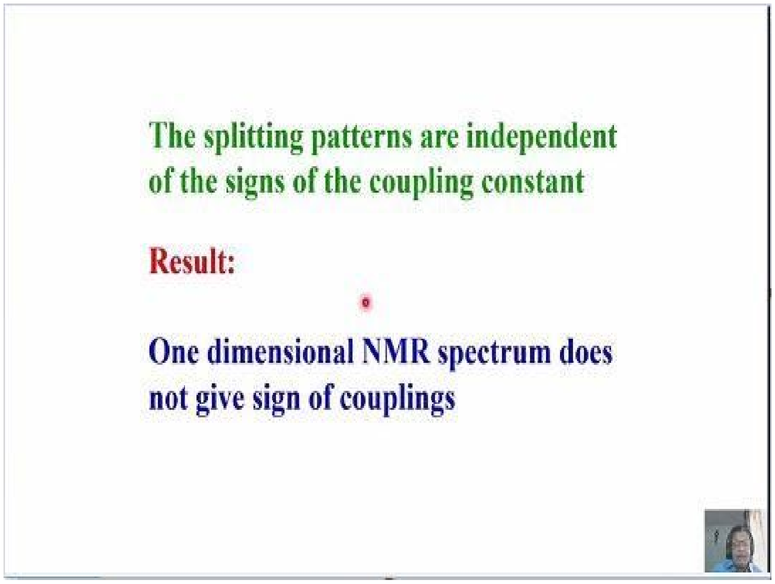

The splitting patterns are independent of the signs of the coupling constant

Result:

One dimensional NMR spectrum does not give sign of couplings

Of course the splitting pattern is independent of the sign of the coupling. Please remember that splitting pattern is independent of the sign of the coupling. So, one dimensional spectrum as a consequence, will not give you idea about the sign of the coupling. Please remember, one dimensional spectrum will not give you information on this sign of the couplings.

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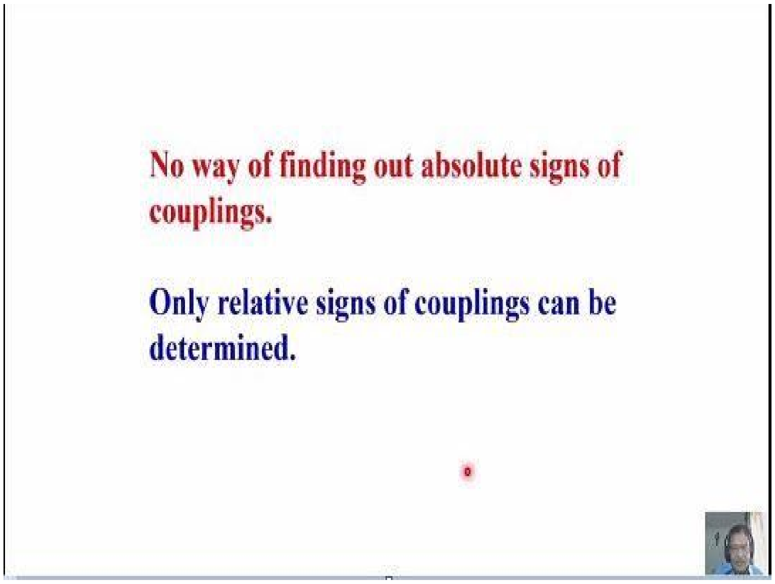

No way of finding out absolute signs of couplings.

Only relative signs of couplings can be determined.

But there are some other experiments we can do, we do not get the absolute sign of the couplings, but we can find out the relative signs of the couplings. You know what it means, I already told you one bond JCH which is positive, if I have a spectrum with carbon proton are coupled. I measure couplings, I know one bond JCH is positive. With respect to that, I can measure this signs of other couplings, in some experiments, it is possible.

So, it means, I will not be able to find the absolute sign of the coupling, in the NMR spectrum. Only I can get the relative signs of the couplings, this is the first point. second, spectrum is remains in variant with the change in the sign of the couplings. So, one dimensional spectrum cannot give information on the sign of the couplings, and for this you need to do some special 2 dimensional experiments.

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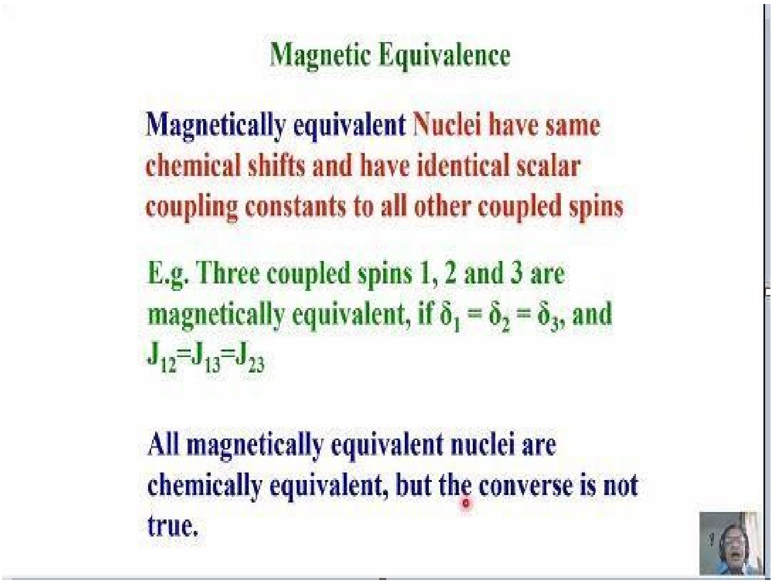

Magnetic Equivalence

Magnetically equivalent Nuclei have same chemical shifts and have identical scalar coupling constants to all other coupled spins

E.g. Three coupled spins 1, 2 and 3 are magnetically equivalent, if $\delta_1 = \delta_2 = \delta_3$, and $J_{12}=J_{13}=J_{23}$

All magnetically equivalent nuclei are chemically equivalent, but the converse is not true.

Now before we go further for analysis of the spectrum. So, far I was talking to you about chemically inequivalent protons couplings, where 1 proton is coupled to 2 protons, 3 protons and we have arrived at the family tree way of multiplicity pattern. But there are examples, where there are chemically equal groups of spins will be there. For example, the will be a CH3 group, there will be a CH2 group present in the molecule, or it may be CF3 group with a 3 fluorines equivalent like CH3 may be present, CF2 may be present. Like that some groups could be there, group of chemically equivalent spins may be there.

That also we need to understand to get the information about the splitting pattern. And before that, remember when I introduced chemical shift, I told you about chemical equivalence, based on the symmetry operation. I wrote symmetry axis and said this proton is equivalent to this, this proton is equivalent to this in chemical shift. But it was there in that slide, I also told you there is a J coupling information. It was at the bottom, I highlighted and said I will discuss this later.

That is the thing now we have to discuss. In the chemical equivalence the chemical shifts are equivalent. Now, think of a situation you have a molecule, may be there are molecules which are chemically equivalent, sorry the spins which are chemically equivalent. But, there are several spins which are coupled among themselves. You understand the question? The molecule chemical shifts may be equivalent for certain protons, but it may so happen, the couplings may also be equal.

But why it cannot happen, it can also happen, why should it not happen? There is a possibility, in addition to chemical shift, J couplings can also become equivalent among coupled spins in some cases. Then, we bring in another term called magnetic equivalence. In the chemical equivalence, we discuss only chemical shift being equivalent based on the symmetry operation, but in the magnetic equivalence, in addition to chemical shift J couplings also will be equal.

This is the example we will look at it. So magnetically equivalent nuclei have all the chemical shifts are same. In addition to that, they have identical scalar coupling constants, to other coupled spins. Very important statement. So, in the case of chemical equivalence, the chemical shifts only were equal. But the magnetically equivalent nuclei have same chemical shifts, they are equivalent; at the same time, couplings to other coupled protons are also same. That is magnetical equivalence.

Say for example, I have 3 spins. Now I will take the 3 spins, 1, 2 and 3. Now what is happening is J12, in this case may be , for all the 3 protons let us assume they have same chemical shift, The chemical shift are same. It has to be chemically equivalent. I take the highlighter, now we see what happened here. So, now 3 protons are there, this proton, this proton and this proton, are all having same chemical shifts, I call it delta1, delta2, and delta 3. Now, I also say coupling between 1 and 2, J 12; coupling between 1 and 3, J 13; and coupling between 2 and 3, J 23. I would say all are same. This information was not told to you before when I discussed the chemical shift or chemical equivalence.

Now I discuss magnetically equivalence, in addition to chemical equivalence I am also telling you, they are magnetically equivalent, because their couplings are also same. This a very important information. So, now the logic is simple all magnetically equivalent nuclei are chemically equivalent. Remember, all magnetically equivalent nuclei are chemically equivalent. Whereas, converse is not true. If I take all the magnetically equivalent nuclei like this one, delta1, delta 2, this one is there. That means, they have to be invariably chemically equivalent, but if only this is in equivalent, it need not be equivalent, that is the reverse case, that is chemically equivalent. So, concept is remember, very simple. All magnetically equivalent spins are invariably chemically equivalent, but all chemically equivalent spins need not be magnetically equivalent. This an important point. You must understand.

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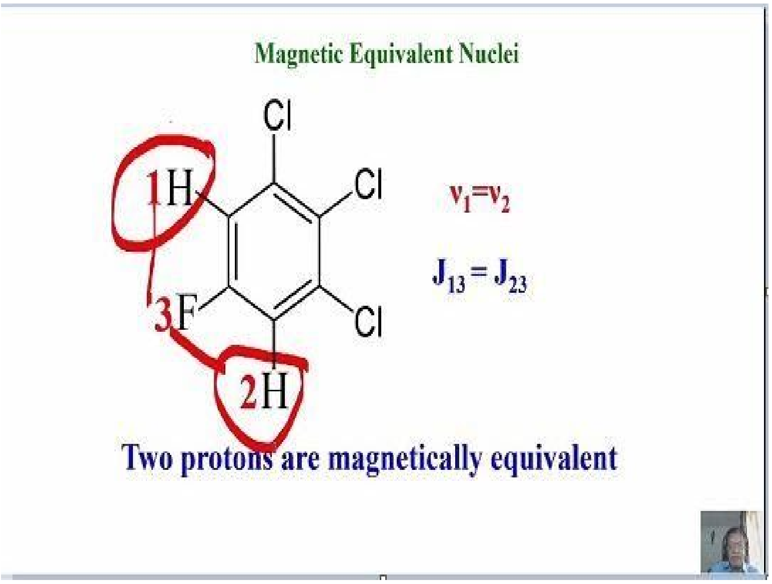

Magnetic Equivalent Nuclei

$\nu_1 = \nu_2$

$J_{13} = J_{23}$

Two protons are magnetically equivalent

Now, let us look at the examples of magnetically equivalent spins. Look at this molecule does it have a symmetry axis? If you look at it, there is a symmetry axis here, along this axis. So, chemical shift of 1 is equal to chemical shift of 2. v1 = v2. what is coupling? this coupling is equal to this coupling J13 = J23. What does it mean? Chemical shifts are also same, coupling of this spin with all other spins are also same. That means, these protons are magnetically equivalent. You understand these protons are magnetically equivalent.

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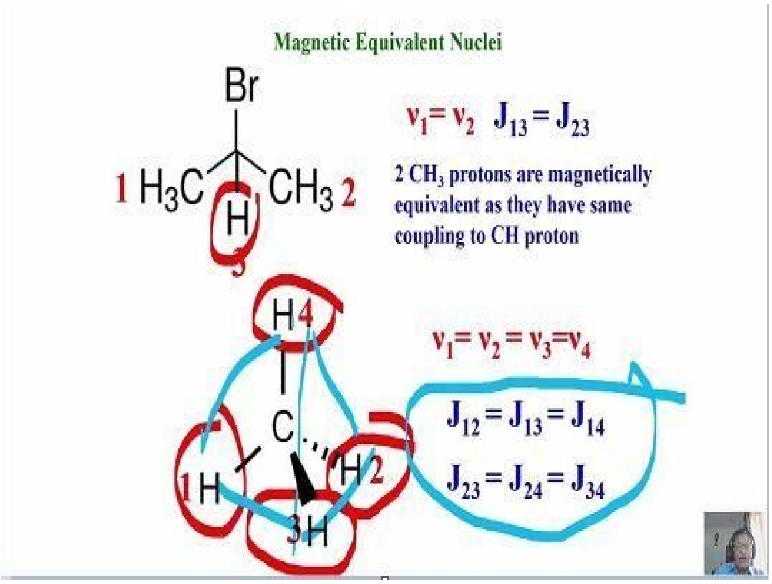

Magnetic Equivalent Nuclei

$\nu_1 = \nu_2$ $J_{13} = J_{23}$

2 CH_3 protons are magnetically equivalent as they have same coupling to CH proton

$\nu_1 = \nu_2 = \nu_3 = \nu_4$

$J_{12} = J_{13} = J_{14}$

$J_{23} = J_{24} = J_{34}$

Now, look at that another example. What about this molecule? There is symmetry axis along this. Now, chemical shift of 1 = 2. All the 3 chemical shifts of CH3 protons are equivalent. Apart from that chemical shift of these 3 protons and chemical shift of these 3 protons are equal. Now, this is different, there are 2 groups of protons, but now look at the coupling of this proton to this, very interesting thing you should observe, the coupling of 2 to 3 and 1 to 3 are all same. J13 = J23. So, that means, two protons are magnetically equivalent, as they have the same coupling to CH proton, in addition to having same chemical shift. These 2 are magnetically equivalent nuclei.

Look at this one. This is a fantastic molecule, it is methane. Now take any protons of your interest, this, this, this or this. All 4 protons have the same chemical shift. See, ν1 = ν2 = ν3 = ν4. That is very interesting thing.

Now, what about the J coupling between this and this, J coupling of this and this, between this and between this, and this, or this and this. Take all the possible couplings here, look at this, J12 = J13 = J14 = J23 = J24 = J34. All the couplings here are equivalent. All 6 couplings are equivalent. What does it mean? For any proton coupling with the remaining 3 protons are same. Any proton you take for 1, 14 ,12 and 13, are same for 4, 14, 34 and 24 are same. Like that all the couplings are same, and all chemical shift are same. So, the methane is an example of a perfectly magnetically equivalent spin system. There are 4 protons that are magnetically equivalent.

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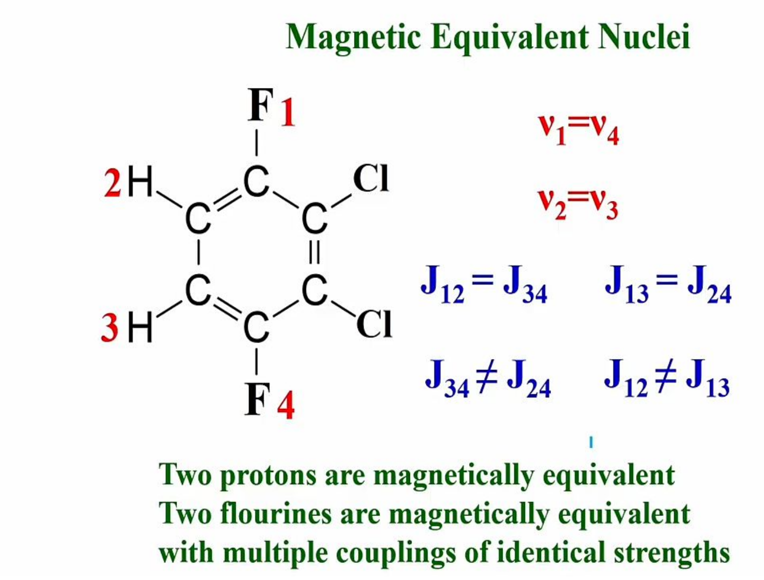

Magnetic Equivalent Nuclei

$\nu_1=\nu_4$

$\nu_2=\nu_3$

$J_{12} = J_{34}$ $J_{13} = J_{24}$

$J_{34} \neq J_{24}$ $J_{12} \neq J_{13}$

Two protons are magnetically equivalent
Two flourines are magnetically equivalent
with multiple couplings of identical strengths

Look at this molecule, this is 14 difluoro and 23 dichloro benzene. Is there a symmetry axis here? yes, one along this, one along this. Two symmetry axis. As a consequence, ν1 = ν4 fluorine 1 and 4 are equal and proton 2 = proton 3. ν2 =ν3. And what about J12? J12 = J34, that is also true. And now, J13 = J24. Whereas, J34 is not equal to J24. Similarly, J12 not equal to J13. What does it tell? these 2 protons are magnetically equivalent. Two fluorines are magnetically equivalent with multiple couplings of identical strengths.

Imagine, there can be a situation where we have magnetically equivalent, but with multiple couplings in the same molecule. Look at this one, I will remove all these highlighters this coupling and this coupling is same. So you can forget about the others, so you take only fluorine, fluorine has 12, 13 and 14; 3 couplings. Similarly, you take this 1, this was 34 and 24 and 14 the 3 couplings , they are identical.

Now go back to proton, proton has 21, 24 and 23 couplings. Similarly, if we take this 3 proton, it has 34 32, and 31 couplings, they are all same. So, that means the 2 protons are magnetically equivalent with different coupling strengths, multiple coupling strengths of identical magnitude. This proton has multiple couplings, this proton has multiple couplings, but the coupling strength though they are different, it is same when you consider this proton and this proton.

You understand what I am trying to say. Here J12 = J34, no problem. Similarly J13 = J24. There are 2 different types of couplings, but they are same. similarly, you can understand, 2 protons are magnetically equivalent, and 2 fluorines are also mechanically equivalent, and with different couplings.

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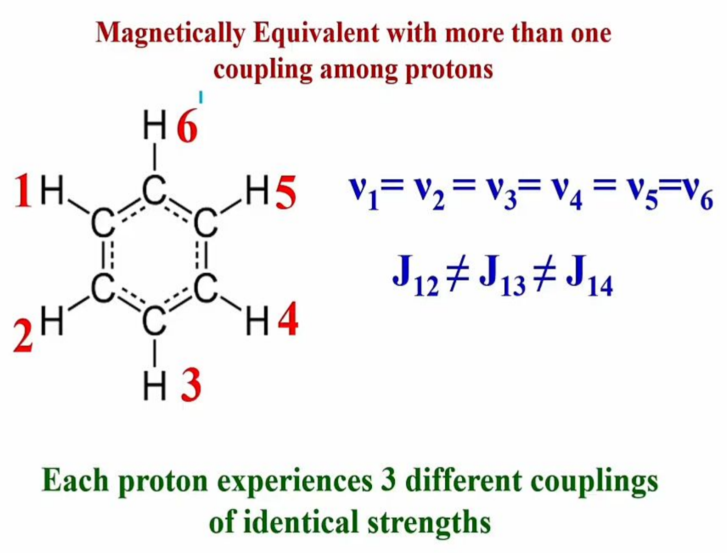

Magnetically Equivalent with more than one coupling among protons

$$\nu_1 = \nu_2 = \nu_3 = \nu_4 = \nu_5 = \nu_6$$

$$J_{12} \neq J_{13} \neq J_{14}$$

Each proton experiences 3 different couplings of identical strengths

What about benzene? it is a very simple molecule, well known. In chemical shifts I have told you, in benzene all 6 protons are chemically equivalent, all 6 protons resonate at the same position and you take the benzene NMR, proton NMR or even carbon 13 NMR, does not matter, you get a single peak, only 1 peak. That means, the chemical shifts are same, ν1=ν2 = ν3 = ν4 = ν5= ν6. see all chemical shift are same.

But what about their coupling strengths? Remember now J12 is not equal to J13, because this is 3 bond coupling. This is a 4 bond coupling, and this is 5 bond coupling. So, J12 is equal is not equal to J13 is not equal J24. Any proton you take, this ortho coupling, meta coupling and para coupling, each proton experiences 3 types of couplings, ortho, meta, and para. Each of the 6 protons have 3 different couplings. But nevertheless, ortho coupling, para coupling, and meta coupling for all the protons are identical.

This ortho coupling is same as this ortho coupling coupling, same as this, same as this, same as this. Similarly, this meta coupling, this meta coupling, this meta coupling, are same. Similarly, this para coupling, this para coupling and this para coupling are same. So, what does it mean?

This is a situation each proton experiences has 3 different couplings of identical strengths, each of these protons. So all 6 protons have same chemical shift. Each of them experience 3 different couplings of identical strengths. This is what is another example of magnetically equivalent spins, with multiple couplings. This is the magnetically equivalent spins with multiple couplings.

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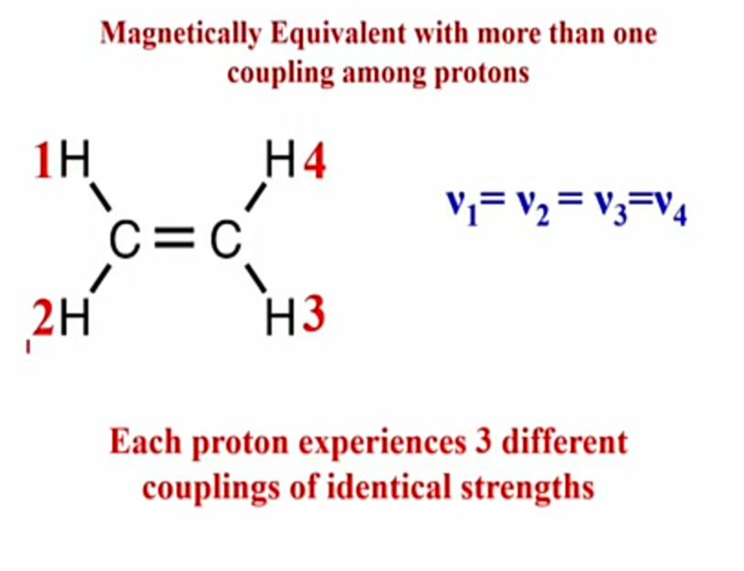

Magnetically Equivalent with more than one coupling among protons

$\nu_1 = \nu_2 = \nu_3 = \nu_4$

Each proton experiences 3 different couplings of identical strengths

Now, in this case what happens? This is ethylene. There is a perfect symmetry along this axis. Now, I can write 1 axis here 1 axis here. This proton is equal to this proton, and this proton is equal to this proton. And similarly, this is same, this is same, this is same. All protons, because of the symmetry consideration are chemically equivalent. ν1 = ν2 = ν3 = ν4. But let us see what are the types of couplings we see. This is a 2 bond coupling germinal, this is three bond coupling vicinal, 1 2 and 3; this is 3 bond coupling trans. 3 bond Vicinal coupling and 3 bond trans coupling, but all are of different strengths. This germinal coupling is different than this vicinal coupling, this vicinal cis coupling and this is visual transcoupling, they are not same. Again it is same for each of these protons, this has again germinal, vicinal and trans, this has again geminal, vicinal and trans. And this has again germinal, vicinal and trans. And we see each proton have 3 different couplings of identical strengths.

So, as a consequence what happens is J12 is not equal to J13; J13 is not equal to J14. Again it is a classic example of magnetically equivalent spins with more than 1 coupling, multiple couplings of identical strengths. This is also magnetically equivalent, but there is one important thing you must observe here. All these are chemically equivalent spins. In these chemical equivalent spins, J coupling is not going to be observed.

I will tell you when we go ahead further. In the chemically equivalent case, J couplings are not reflected in this spectrum. Same if we go back to benzene, benzene gives a single line, but I said there are 3 different couplings, but why are we not seeing multiplicity? Always in chemically equivalent and magnetically equivalent cases, the couplings are not reflected in this spectrum; you will not see the couplings, they disappear even though they exist. Not that coupling is 0, here ortho, meta and para couplings are present. They are not 0. But only thing is you do not see them in this spectrum. Same here, in this example. So, but then question is, how do I know what are these couplings? Here also I said we get a single peak. Ethylene you know comes at 5.29 ppm, in one of the chemical shift slides I showed you. All protons are chemically equivalent comes at 5.29 ppm. With 1 peak how did I measured all the couplings. This is a fantastic example to tell you how we can get the couplings in chemically or magnetically equivalent spins.

We will discuss this later, after a certain number of, or maybe after 1 class, 2 class, I will take specific examples, how we can get the couplings in chemically equivalent spins. We will come to that later. At the moment. Do not worry, but remember the 3 different couplings are present, you do not see any spectrum. And 3 and 4 chemical shift are also identical. So it is a magnetically equivalent spins with multiple couplings. Now, with this knowledge, let us go and look at the multiplicity of different spin systems. How they the couple, when they are chemically equivalent, what will happen to the splitting pattern. It is a very interesting thing you must try to understand.

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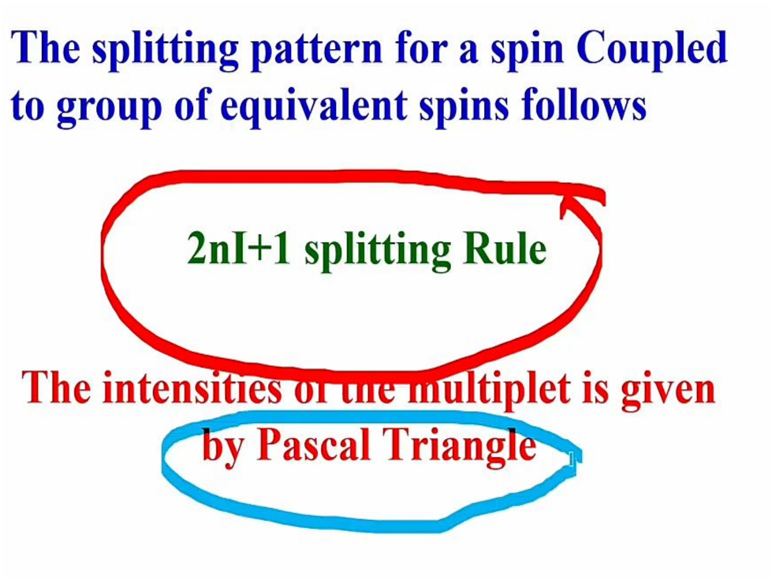

The splitting pattern for a spin Coupled to group of equivalent spins follows

2nI+1 splitting Rule

The intensities of the multiplet is given by Pascal Triangle

Remember in the slide when I was briefing you the salient points of scalar couplings, I made one statement, that splittings among the group of equivalent is given by 2nI+1 rule, I said I hope you remember, I said splitting among this thing is given by 2nI+1 rule. And I also said intensities of these things are given by Pascal triangle; intensities of multiplets are given by Pascal triangle. That is a very interesting, this is a point you remember, this is important statement.

If you have CH2 group, they are chemically equivalent, the 2 protons, and if I have the CH3 group, all the three protons are chemically equivalent, but CH2 protons can couple to CH3 protons, similarly CH3 protons can couple to CH2 protons. In both the cases the splitting is shown by 2nI+1 rule. And what is intensity pattern? it is unlike in chemical inequivalent spins where the they are of equal intensity, here the intensity patterns are different. And that is given by Pascal triangle. Remember, this one. That is given by Pascal triangle.

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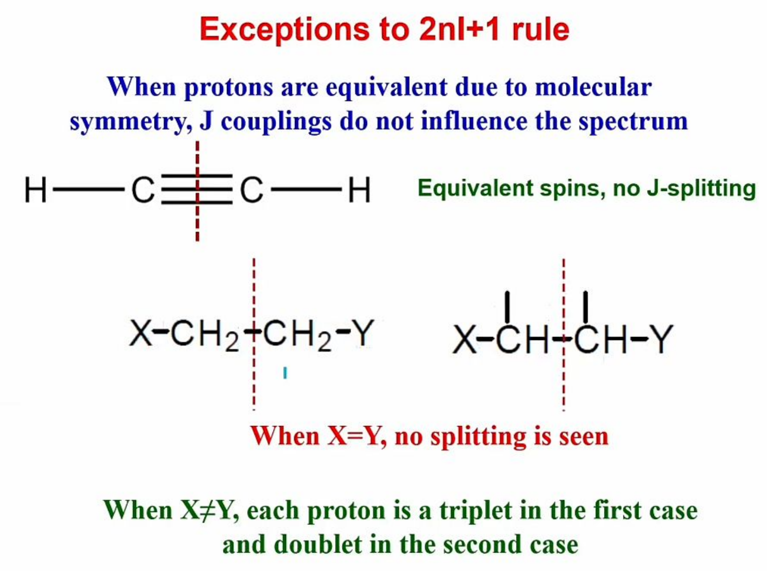

Exceptions to 2nI+1 rule

When protons are equivalent due to molecular symmetry, J couplings do not influence the spectrum

Equivalent spins, no J-splitting

When X=Y, no splitting is seen

When X≠Y, each proton is a triplet in the first case and doublet in the second case

We will see what it is. But there are exceptions for 2nI+1 rule. onsider a molecule like this, there is a perfect equivalence among the spins, this is equivalent to this, and then this is equivalent to this, it will not give rise to the coupling with this. This will not couple to this one, same way this carbon this will not couple to this carbon. In the case in equivalent case when there is a symmetry J couplings do not influence the spectrum. You understand, this is exception for 2nI+1 rule look, at this one.

If X and Y are different, then this environment is different, and this environment is different. As a consequence, what is going to happen? This proton splits this proton, because of coupling with this. This protons splits because of this, because X and Y are different. There is no chemical equivalence. On the other hand, if X = Y. In this case, or in this case; No problems. When X = Y, there is no coupling at all. You do not have to worry about anything, simply say there is a symmetry and in this molecule this proton cannot interact with this proton, there is no coupling, it is not seen in this spectrum. So, this is the example of cases, where you will not be able to see the coupling among equivalent spins, by just by applying 2nI+1 rule.

Supposing X is not equal to Y here, what I get if X is not equal Y here , what type of splitting I get I will now explain to you.

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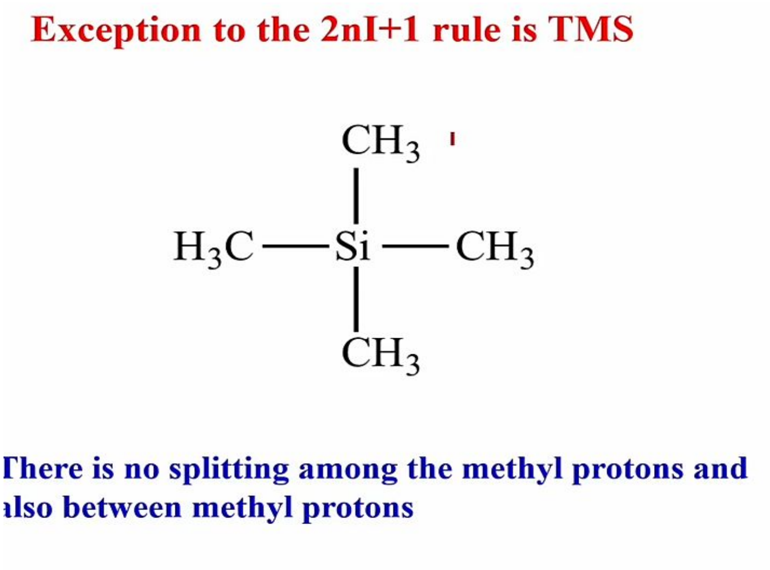

Exception to the 2nI+1 rule is TMS

There is no splitting among the methyl protons and also between methyl protons

Now, look at the tetramethylsilane molecule. It is a very simple molecule, all of you know that when I discussed chemical shift itself. Remember, when I discuss chemical shift, I explained to you this CH3, this CH3, this CH3 and all CH3s are chemically equivalent. And the protons of this CH3 group are also chemically equivalent, that means all the 12 protons we have 12 protons, here you know. All the 12 protons of tetramethylsilane are equivalent, chemically equivalent and also magnetically equivalent. Coupling between this CH3 to this CH3, this to this, this to this, this to this, are same. You will not see the effect on this spectrum. That is the, another example to say 2nI+1 rule do not apply here. This cannot split because of this under 2nI+1 rule. This cannot undergo splitting because of this under 2nI+1 rule. These are the classic examples to show, there are exceptions for the 2nI+1 rule.

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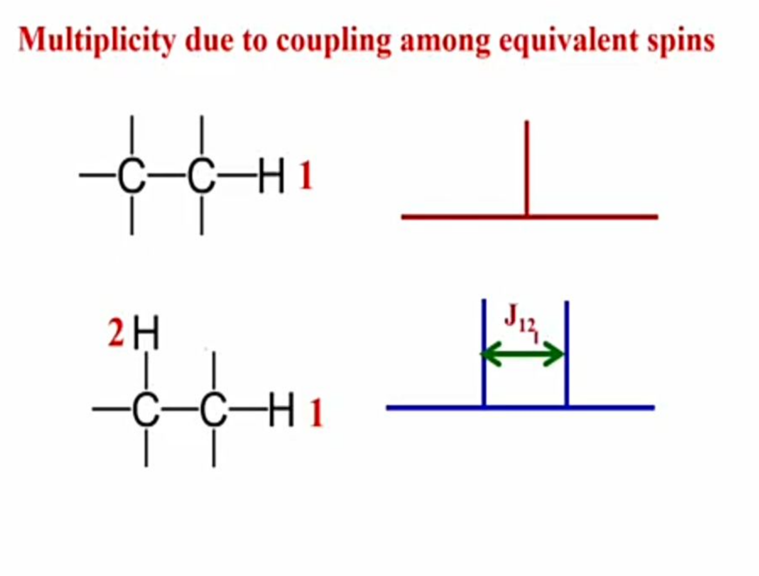

Now, with this idea in mind, let us start looking at the multiplicity pattern due to coupling among equivalent spins. This is now deviating from other way, in other case we are simply seeing only 1 proton, one spin coupling to other single spin. So, the family tree approach was followed, where one becomes 2, to becomes 4. That was the base to understand multiplicity and at the end all will be of equal intensity, but now, let us see what happens when equivalent spins are there, when equivalent spins are there, things are different.

Consider an example like this, there is only 1 proton, you get only 1 line. Now consider a situation 1 proton is coupled to another proton, you get 2 lines. Consider a situation. Ofcourse this coupling is J12, it is well known when 2 protons are coupled we get the doublet for this and also doublet for this, this we have been discussing.

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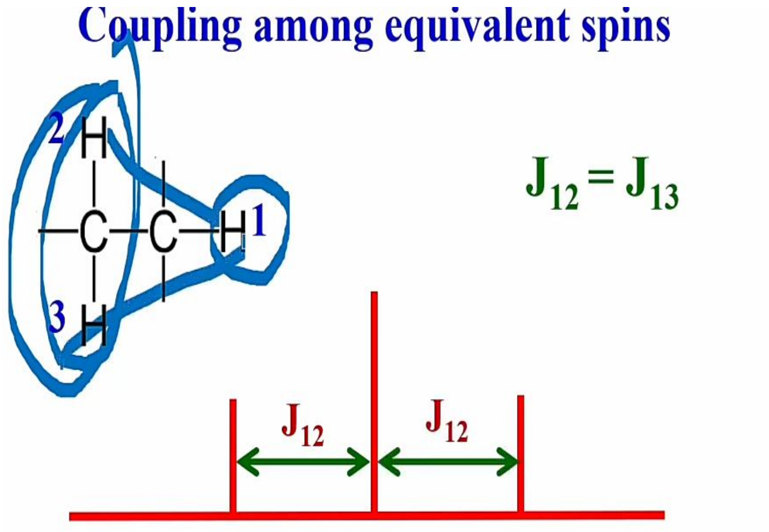

Coupling among equivalent spins

$J_{12} = J_{13}$

Now interesting thing is. Look at this molecule, in this case there is a perfect symmetry on this axis, that is this coupling and this coupling are same; J12 = J13. then this undergoes splitting because of this and this together. Similarly these 2 protons will undergo splitting because of this proton. you understand what I am trying to say, this proton and this proton splits this one together and these 2 together are split by this proton.

Now, let us see what happens. This is an example to show that J12 = J13. It is a chemically equivalent spin. It is called CH2 or equivalent groups. In this case, simply I will say proton is coupled to CH2. That is all; Look at this, it gives me a triplet. When I look at the proton 1, the proton 1 when it is coupled to 2 equivalent protons gives me a triplet. How? We will understand how it goes; and this separation gives me J12 or J13, does not matter, both are same, because I have written the equivalent relation here. So that is a situation.

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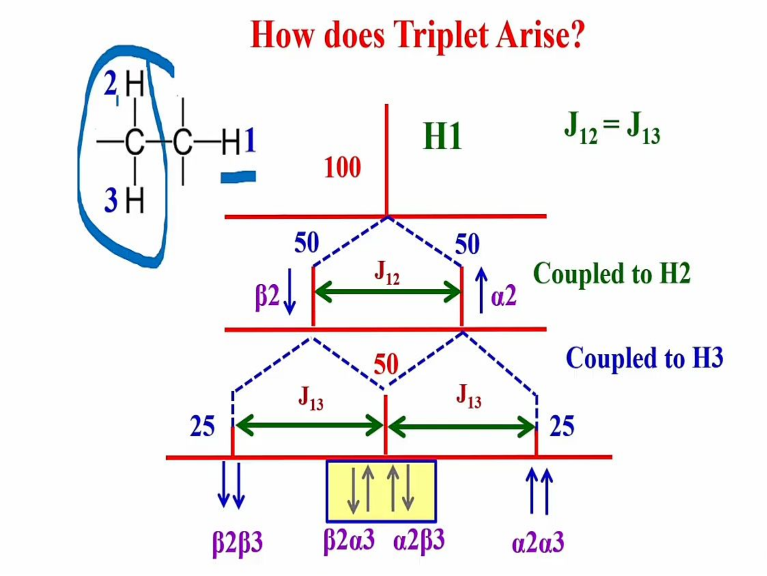

How does this triplet arise is something interesting. Let us understand this no;w how does the triplet come? I will start with the simple case, without any splitting between these 2, this will give a singlet. Now I will bring the coupling to proton 2. Remember the family tree it becomes doublet of equal intensity. Now the intensity has come down by 50 , 50, it is 50%; divided you know. the distribution of intensity between 2 members of the family.

So intensity became 50 50. And this coupling is J12. Now, I will bring in the coupling to proton 3, this is alpha beta spin states of proton 2. That is why we have 2 orientations and doublet. Now, I will bring in the coupling to proton 3, proton 3 also undergoes coupling and each line split into doublet. So what is intensity? This is 25, here 25, here 25 here and another 25, because this is doublet has 25, 25 intensity; this doublet has 25, 25 intensity. This will overlap and gives rise to 50 intensity.

You understand now, in this case, this is a 50% intensity because 2 lines of this intensity are overlapped here. Why do they overlap? because the couplings are same; J12 = J13. If J12 is not equal to J13, you could got 4 peaks; like a family tree approach what we did, but because of equivalence, the central two peaks of equal intensity are overlapped. So, you now understand. It was 100 intensity, became 50;50 because of coupling with this proton, and each of them become 25, 25, 25 and 25. These 2 central peaks overlap and total intensity becomes 50.

What is it intensity ratio now, 1 : 2 : 1. You understand, do not get confused. Now the intensity ratio is 1 : 2 : 1. This is when 2 equivalent protons are coupled to a single proton. You get 1 : 2 : 1 intensity ratio. Now, this can be understood with a different logic, why does this logic? these 2 correspond to beta beta orientation, and here there are 2 possible orientations alpha beta, beta alpha, they overlap and give rise to 2 intensity. Now, this corresponds to alpha alpha, this is only 1 intensity.

See, this is one intensity, these 2 are same overlapped and twice the intensity and this is one intensity. As a consequence, a triplet intensity with ratio of 1 : 2 : 1 is observed. You understand how the triplet comes with an intensity ratio of 1 : 2 : 1, when the 2 equivalent protons are coupled to a third spin. Now, the question is what happens to this proton, I will ask you what happens to these 2 protons, when it is coupled to one, all of you should know. This is equivalent as far as I am concerned and I observed a single peak, because these 2 are equal; chemically equivalent spins.

And now this is third spin, just it will become a doublet, nothing more. Because these 2 are indistinguishable, there is only 1 peak. You can consider this as a single spin, a compound spin. When it splits with this one, this proton, becomes a doublet. So, in this case, if I have a situation like this. a molecule like this, this will become a triplet and this will become a doublet. So if I take the NMR spectrum of this molecule, I will get a triplet and I will get a doublet. That is the total spectrum. All of you, I hope you understood.

Triplet comes because of 2 central peaks overlap, and that is possibility we have 2 alpha beta and beta alpha identical energies overlapped. And this is alpha alpha orientation, and this is beta beta orientation. So this is a simple example to say, when do you get it triplet when any any of the proton or group of proton, does not matter, it may not be single proton, it may be CH3, CH2 and when it is coupled to two equivalent spins CH2, the splitting pattern will always be a triplet for this one.

Remember, this will be always be a triplet. This is what I just wanted to tell you about this, we will continue with multiplicity pattern how it comes for other spin systems, like when we have

CH3 coupled. When we have CH2, CH 3 coupled, how it comes everything later. what happens when 2 CH2s are coupled or when on CH2 or 2 CH3 are coupled, varieties of examples. We have a couple of more examples we will take up and understand how this splitting arises in the case of chemically equivalent spins. So we will do that in the next class. Right now, I am going to stop.