

**One and Two dimensional NMR Spectroscopy: Concepts and Spectral Analysis**  
**Prof. N. Suryaprakash**

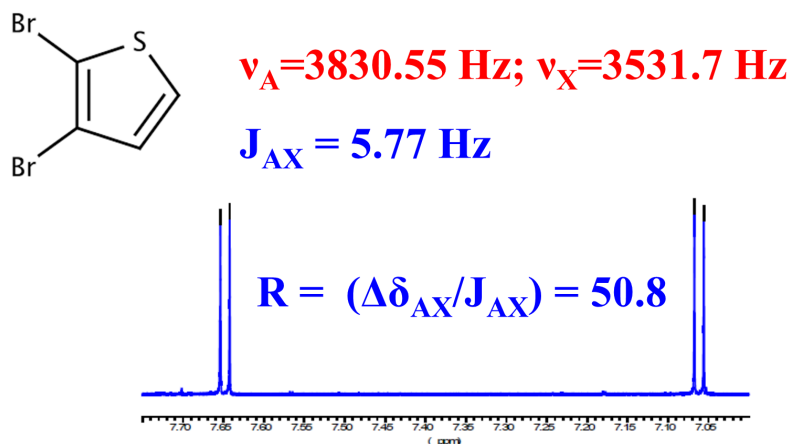
**CSIR Emeritus Scientist, Solid State and Structural Chemistry Unit**  
**Indian Institute of Science – Bengaluru**

**Lecture 18 : Energy levels of two and three coupled spins**

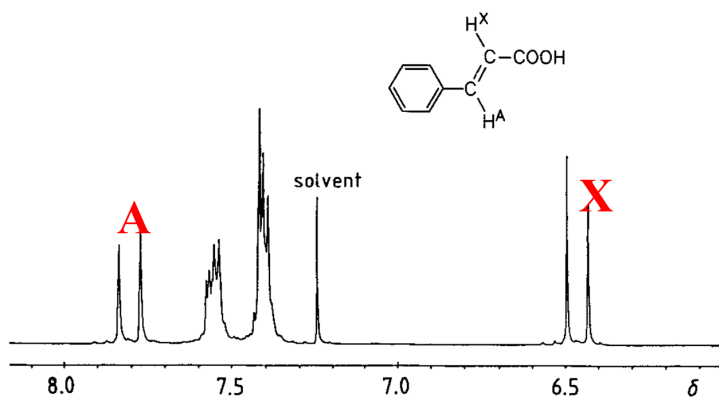
Welcome all of you for today's class. In the last class, we discussed extensively about the coupled spin system. We understood the difference between strongly coupled and weakly coupled spin system. And also, I discussed a lot about Pople nomenclature, in the sense, when the spins are strongly coupled or weakly coupled, it can be characterized by certain limitations. For example, weakly coupled spin systems are called AX, AMX, AMPX, etcetera. Whereas, the strongly coupled spins are identified as AB, ABC, ABCD, etcetera. For the strongly coupled spins, the the alphabets next to each other in the Roman alphabet order is defined. Whereas, for weakly coupled, the alphabet which is far away in the alphabet order is taken into account. Then it represents weakly coupled systems. Spins referred by alphabets next to each other are called strongly coupled. That is how it goes. And I took several examples to discuss the strongly coupled spectra, weakly coupled spectra, molecules which are strongly coupled and weakly coupled. When there is chemical equivalence, I said we can use prime notation. When there are groups of spins that are chemically equivalent like CH<sub>2</sub>, CH<sub>3</sub>, we can use subscript notation. And then Write down the Hamiltonian and diagonalizing the matrix, get the Eigen values, we can get frequencies, we can get the frequencies of transitions. I got four transition for two coupled-spin system. and then we can get the transition difference in the frequencies, between different as per the selection rule, we found out there are four transitions, in weakly coupled AX spins case where two for A and two for X are there. And from the center of the chemical shift each peak moves on either side by J/2 that is what we understood. And I said for a weakly coupled spin case or for two coupled spins are there you can get maximum of four transitions.

Let us continue further today and see what is going to happen in other spin systems. We will now consider the example of N coupled spins. For N coupled spins there will be total of  ${}^{2N}C_{N-1}$  transitions. For example, if I take three inequivalent coupled spins we should get  ${}^6C_2$ , that is 15 transitions. If there are 4 spins maximum you should get is 56 transitions. Of course, by a first order approximation, and you know by a family approach we have been discussing, I said for three spins, each spin will give rise to four transitions and there could be maximum of 12. Why then 15 is coming into the picture? Remember once I said there are combination transitions. Then there will be three more transitions which does not give information about the chemical shifts which comes at with sum or difference of the chemical shifts. The J coupling information is not be possible to get

from that. Also similarly, four spin also we have maximum of 56 transitions and most of these transitions are highly redundant. In the sense, for example, if I take three spins there will be 12 transitions and at the site of chemical shift of each of them there will be four transitions and that gives you two coupling information. We have maximum of three couplings, but at each chemical shift we can get two coupling information. That means there is a redundant information. So, the single quantum NMR spectrum are generally highly redundant. So, only few of the transitions are just sufficient to get the chemical shift and J coupling information.

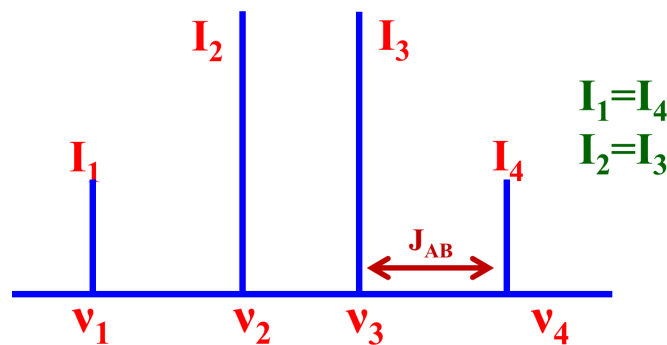


So, this is a typical example of an AX spin case where chemical shift of A and X are like this, and the J coupling interaction is 5.77 Hertz and if you take the ratio it is about 50.8. Clearly it is a weakly coupled AX spin we get four peaks of equal intensity, but still you see there is small intensity difference; you do not have to worry about that. That deviation says there is a minute strong coupling character, but for all practical purposes this can be treated as a weakly coupled two spin case.



A realistic example is like this where a molecule like this is there and you can see two transitions here for X and A. They are not of equal intensity. In principle they have to be equal intensity. I consider hypothetical example of an AX case for a heteronuclear spin here proton and fluorine are taken into account, mind you, proton and fluorine peaks will not come at the same frequency. They are coming at different frequencies, that we know. Proton in a 500 megahertz spectrometer resonates at 500 megahertz, whereas fluorine resonates at 470 megahertz. Just for the sake of illustration both of them are plotted in the same graph. This is proton, this is fluorine. You see in this theoretical plot, all the lines are of equal intensity. This separation gives you J coupling between proton and fluorine. Again this coupling this separation gives you coupling between proton and fluorine. This is a typical example of hypothetical AX case for a heteronuclear two coupled spins. And each peak can be assigned to a particular transition. For example, we have been discussing depending upon the selection we can find out from the four Eigen states we get, we can find out the frequency of transitions. For example 1 to 2 and 3 to 4 correspond to X transition and 1 3 and 2 4 correspond to A transition; this is X transition this is for A transition. And easily we can assign that.

And if you go even further we have another example of strongly coupled two spins. It is AB. Earlier it was AX now it is AB. As I said the two letters are close in the alphabet means they are strongly coupled spins. And in the case of the strongly coupled the chemical shift A is not equal to B that is they are two different chemical shifts, but  $\Delta\delta$  difference in the chemical shift is approximately equal to J coupling, and J coupling is non zero in this case. And if you think of a strongly coupled spins two spins you cannot get heteronuclear AB, because the chemical shift separation is of the order of megahertz several megahertz compared to coupling of the few hertz. As a consequence the heteronuclear AB spin system is impossible to get. You always deal with only homonuclear AB spin system. Now how does the spectrum come? This is how the spectrum appear. It is hypothetical AB spectrum pattern.



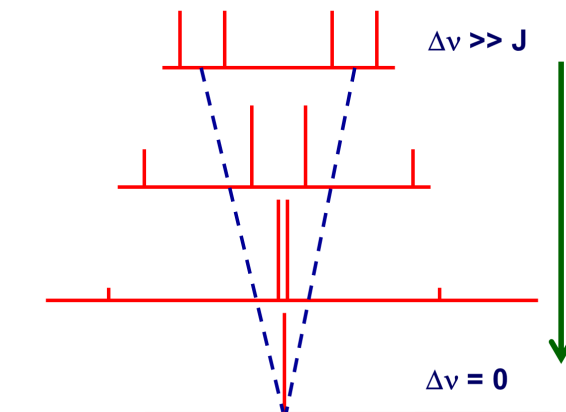
And you see two central lines are of equal intensity two outer lines are of equal intensity, but all the four lines are not exactly equal unlike what you see in the AX spin case. But of course, there will be always a strong coupling effect. In this the roof you can see this is tilted like this, that shows there is a roof effect. Roof effect will be there in most of the cases in strongly coupled spin systems. And of course, without going to the details, which have been already discussed in many of the earlier two courses, you can find out from the intensity this coupling and the separation has to take into account the transitions and by using a simple equation like this

$$\Delta\nu = \sqrt{(\nu_1 - \nu_4) * (\nu_2 - \nu_3)}$$

gives you the J chemical shift be obtained by the frequency of

And AB system gives centro symmetric four peaks. Two central peaks are of identical intensity and two outer peaks are of identical intensity and regardless of how strong the coupling, the difference in the frequencies the outer line separation always gives rise to J coupling. For example, I have four peaks here and outer two lines separation always gives rise the J coupling, whatever be the strength of the interaction.

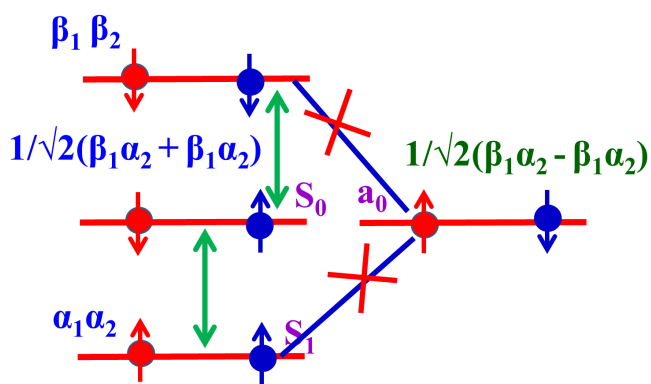
AB coupled spin system can have two limiting cases. One is in a situation where this is difference in delta delta by J is enormously large. Of course, AB can go to AX and if it is extremely small or in a situation where the chemical shift difference is 0, then AB can become A2. Remember AB can be taken to AX by going to higher magnetic field or also if you go to very very low magnetic field and if the chemical shift difference becomes 0 it can become A2 and remember AX to AB AB to A2 transition is always continuous. Smoothly you can keep changing it. So how it goes I will show you in this plot.



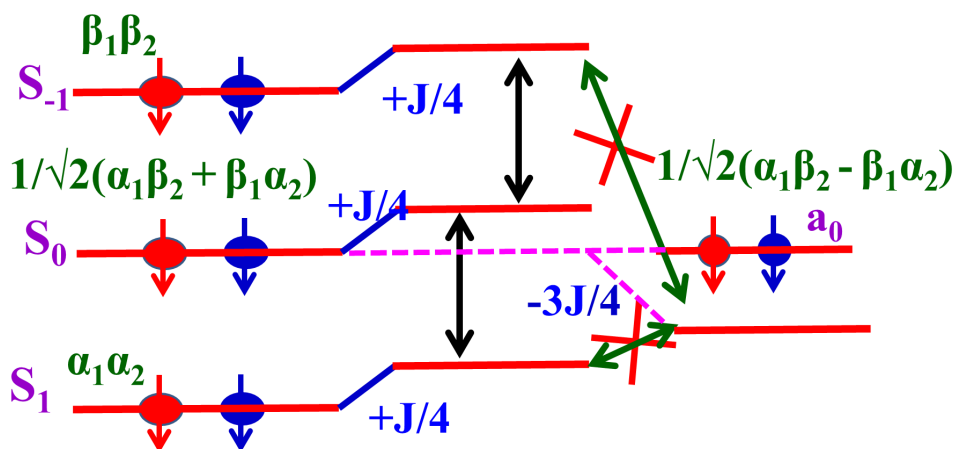
For example, this is AX case where four lines are of equal intensity and in this case  $\Delta\nu$  is very much larger than  $J$  let us find out the situation what happens as  $\Delta\nu$ , the chemical shift difference between two spins A and B, becomes smaller and smaller or almost comparable to  $J$  coupling. You see what is happening? You can see that. You can trace the curve. The outer lines start moving away and it gets reduced in the intensity and inner lines increase in intensity. In a situation when chemical shift difference become equal to 0 then both these lines will overlap. And outer lines completely disappear and this is the transition from AX to A2. Remember AX can go to AB and when the chemical shift difference becomes 0 it can go to A2. This is an example how it goes of course, not only the chemical shift, you can also vary the magnetic field you can find out what happens. This is an example to show  $\Delta\nu$  we keep on reducing it and how it is happening.

What is an A2 spin system? A2 spins are very very strongly coupled AB itself is strongly coupled and A2 is even more strongly coupled. In the case of A2 what will happen is the chemical shift of A1 is equal to delta of A2, The difference is 0;  $\Delta\nu$  is 0. And  $J_{A1A2}$  can be equal to 0 or need not be equal to 0. And in the case of the homonuclear A2, always you can go to get the homonuclear case because chemical shifts are always equal to zero. The heteronuclear A2 is impossible; as similar to AB heteronuclear AB is not possible heteronuclear A2 is also not possible. That is because of large chemical shift difference; the resonating frequencies are megahertz apart.

And what are the transitions you can see in the A2 spin system. Of course, one interesting thing you should understand A2 has four energy states beta beta, alpha alpha, but in the weakly coupled case you have beta alpha and alpha beta, but in the strongly coupled case without going more into the details I can say these are the four spin states. And one of them is beta beta; this is  $1/\sqrt{2}(\alpha_1\beta_2 + \beta_1\alpha_2)$  and  $1/\sqrt{2}(\alpha_1\beta_2 - \beta_1\alpha_2)$  and alpha alpha. The three states are symmetric states and this is anti symmetric state. One of the selection rules of NMR is symmetric to anti symmetric transitions are forbidden. You cannot have a transition from this to this; this to this; or this to this. So, this is a single energy level separated out there would not be any transition. Whereas, from the symmetric there can be transitions from here to here, here to here, it is allowed. So, now let us see what happen to the situation when their coupling is 0.



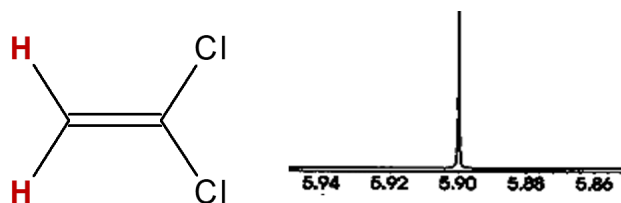
There is no shifting of the energy states as I said only when there is a coupling then the energy levels alpha alpha and beta beta gets shifted up by  $J/4$ ; and similarly alpha beta beta alpha shifted down that is what we have been discussing for weakly coupled. Exactly like this. Now, in this case of  $J_{AA}$  equal to 0, there is no shifting of the energy states. This is the energy level diagram and you have only two transitions of identical frequencies; two transitions of identical frequencies will be there. In that case they will overlap and gives rise to a single peak. And of course, transition from symmetric to anti symmetric are forbidden that is what I said.



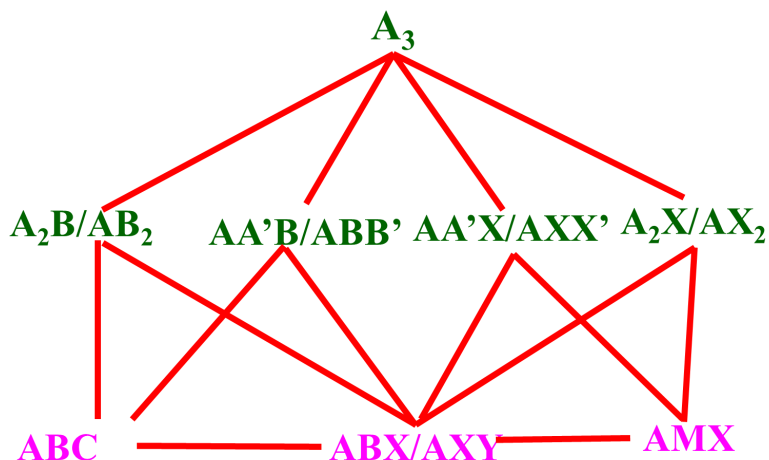
What happens if the coupling is non zero. The same example we discussed for AX case. When the coupling becomes non zero that means,  $J_{AA}$  is greater than 0, of course, it can be less than 0 also, I said non zero. We have again three energy states which are symmetric states and what happens? as I said when there is a coupling, these energy states are shifted up by  $J/4$ ; whereas, anti symmetric energy state is shifted down by minus  $3J/4$ . Remember in the case of AX the alpha alpha and beta beta states shifted up by  $J/4$ ; the alpha beta and beta alpha states both shifted down by  $J/4$ . Whereas, in this example all the three symmetric states are shifted up by  $J/4$ , and the anti symmetric state will come down by  $-3J/4$ . This is an important thing. How you get it? you can work out mathematically quantum mechanically. I am not going to the details of that just for you to understand what is happening when there is a coupling and there is no coupling how many peaks you are going to get. Here also only two transitions are allowed and transition from here to here symmetric to anti symmetric is forbidden. You are not going to see any transitions between these two. So, you have two lines of again identical

frequency. They will overlap and give rise to a single peak. So, whether the coupling  $J_{AA}$  present or not present, in the A2 case you are going to get a singlet. this is what it is.

A simple example of A2 is the tetra chloro benzene symmetrically substituted like this. and these two protons are chemically equivalent and it uses to a 2 spin system and you are going to get a singlet. You understood in principle two protons are coupled; two spins are coupled, you must have four transitions. In the classic example of the A2 because there is no transition from symmetric to anti symmetric we have only two frequencies which are identical and they overlap give rise to a singlet. and it has only two transitions and outer transitions anyway have completely disappeared.

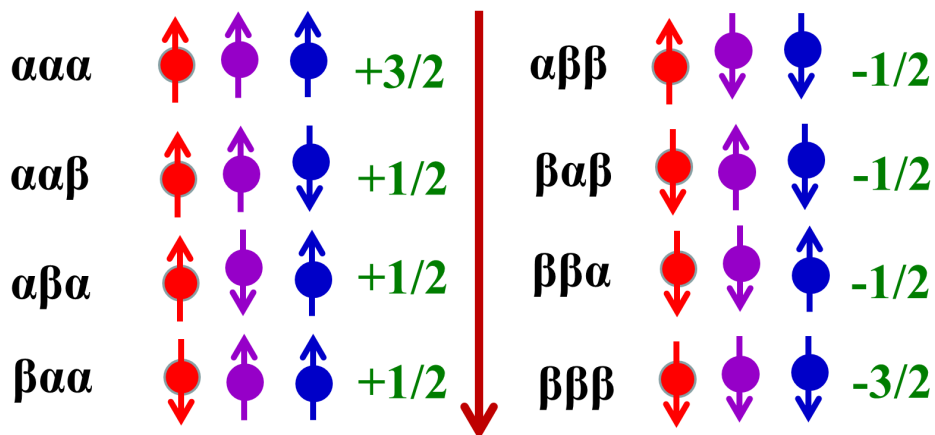


Of course, you may ask me a question what happens  $J_{AA}$  instead of positive becomes negative everything is same, instead of this pushing up all the thing sates will pushed down by  $J/4$  and this one instead pushing down gets pushed up by  $3J/4$ , that is all. Again the transition frequency remains same. This is what happens and this is a classical example of an A2 spin case where there is only two protons are chemically equivalent no J coupling information and only singlet a single peak. So, these are the example of A2. Remember AB gives 4 peaks, of course, they are not of equal intensity 2 central peaks are of equal intensity 2 outer peaks are of identical intensity, but all the 4 are not same. The AX has 4 peaks all 4 of equal intensity, but A2 gives only 2 peaks, 2 transitions which are overlapped.



And of course, if you go to the 3 spin case, you can think of what are the possible combinations. In the 2 spin case you have only 3 possible combinations A2, AB and AX. If you go to 3 spins case you can get plenty of possible combinations. it can be A3,A2B, AB2, AA'B, ABB'. AA'X, AXX', A2X, AX2, ABC, ABX, AXY, AMX. See varieties of combinations you can think of. So, in principle all the spin systems for a 3 spin case depending upon the coupling strength and chemical difference you can define. Nut remember A3 gives only a single peak, whereas, AB2 will give rise to 9 peaks; whereas, AMX is going to give you 12 peaks, ABC gives you 15 peaks and the type of spectrum which you see or the appearance of the spectrun is entirely different, they are not same.

So, this is how we have to understand the NMR spectrum analysis. They are all coupled spin systems; depending upon the strength of the coupling their chemical equivalence or magnetical equivalence, depending upon whether the chemical shift is there or not and what is the difference in the chemical shift and with respect to the J coupling we can have strongly coupled and weakly coupled spin systems, and varieties of nomenclatures we can arrive at. Of course, we do not want to go into the detailed discussion of everything becaus this has already been discussed N number of times.

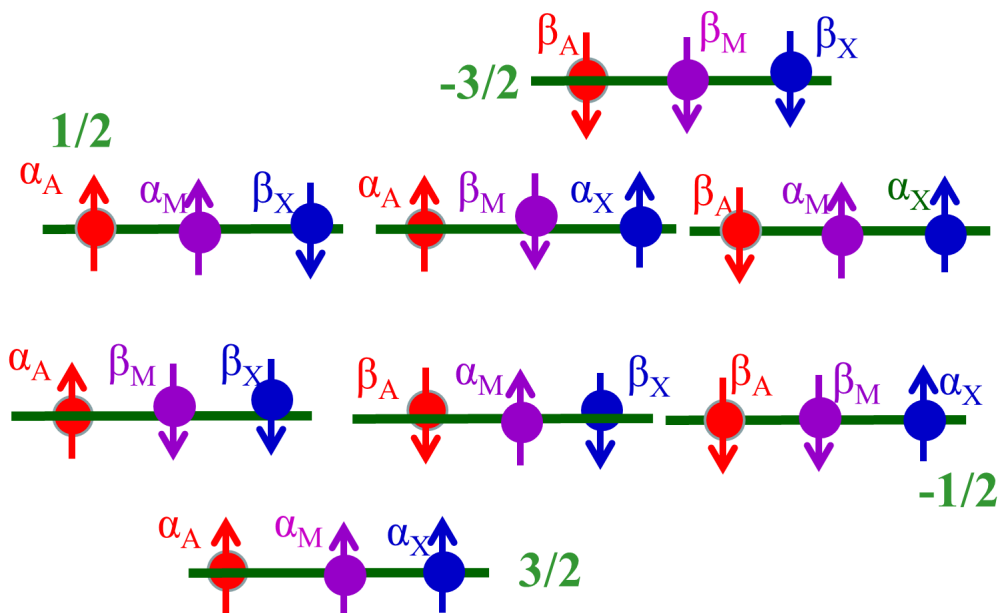


Now, we will see the energy states for 3 spins, weakly coupled. I am taking AMX spin sytem. Of course, we have many possible energy states for the 3 spins. I have already discussed for N coupled spin system, there are  $2^N$  energy states. So, for 2 spin we have 4 alpha alpha, alpha beta, beta alpha and beta beta. For 3 spin it is  $2^3$ . What are the combinations, alpha alpha alpha, 2 alpha 1 beta like this, and in other example we can see 2 beta 1 alpha, and finally beta beta beta. So, there are these possible 8 energy states. And this is my total magnetic quantum number. It is  $3/2$ , this is  $-3/2$ ; this is all  $-1/2$  and this are all  $+1/2$ . So, these are the 8 possible energy states. Of course, we discussed about the possible transitions when I showed you about 3 spin case. For the AMX we will have 4 possible transitions for each spin. For example, X can have like this; and X can have



like 4 transitions, A can have 4 transitions like this; and similarly M can have 4 transitions like this.

So, in the weakly coupled case remember each spin will give rise to 4 transitions, but of course



But of course, we can work out the frequencies like this. I already worked out. But you have to write down the Hamiltonian for this case or for 3 individual chemical shifts are there, 3 different couplings are there. You have to take all this into account and diagonalize the Hamiltonian. You will get 8 X 8 matrix. You have to diagonalize it and get the Eigen values; and these are the Eigen energy states and using these you can get the frequencies. of course, in this case you can find out the allowed transitions. For example, 3/2 to minus 1 is allowed; plus half to minus half is allowed; you can find out what are the allowed transitions. Accordingly take the difference between the energy states which is given.

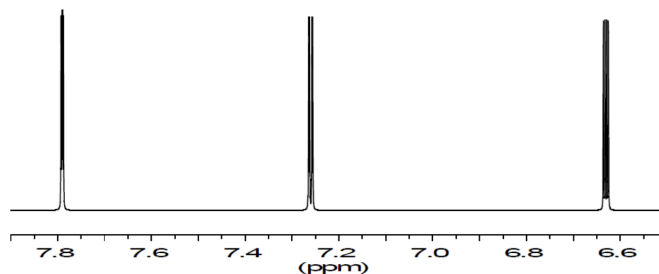
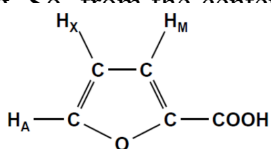
State	(F <sub>z</sub> )	Function	Energy of the state
1	+3/2	$\alpha\alpha\alpha$	$(\nu_A + \nu_M + \nu_X)/2 + (J_{AM} + J_{AX} + J_{MX})/4$
2	+1/2	$\alpha\alpha\beta$	$(\nu_A + \nu_M - \nu_X)/2 + (J_{AM} - J_{AX} - J_{MX})/4$
3	+1/2	$\alpha\beta\alpha$	$(\nu_A - \nu_M + \nu_X)/2 + (-J_{AM} + J_{AX} - J_{MX})/4$
4	+1/2	$\beta\alpha\alpha$	$(-\nu_A + \nu_M + \nu_X)/2 + (-J_{AM} - J_{AX} + J_{MX})/4$
5	-1/2	$\alpha\beta\beta$	$(-\nu_A + \nu_M + \nu_X)/2 + (-J_{AM} - J_{AX} + J_{MX})/4$
6	-1/2	$\beta\alpha\beta$	$(-\nu_A - \nu_M + \nu_X)/2 + (-J_{AM} + J_{AX} - J_{MX})/4$
7	-1/2	$\beta\beta\alpha$	$(-\nu_A + \nu_M - \nu_X)/2 + (J_{AM} - J_{AX} - J_{MX})/4$
8	-3/2	$\beta\beta\beta$	$(-\nu_A + \nu_M + \nu_X)/2 + (J_{AM} + J_{AX} + J_{MX})/4$

You can find out what are the 12 transitions; 4 for A, 4 for M and 4 for X. And you can find out from the center of the chemical shift there will be 2 peaks on right side and 2 peaks on the left side. One peak moves by half of 1 of the coupling other one moves by half of the other coupling. The same thing happens for the left side from the center of the chemical shift. This is true not only for proton A, but also for proton M and for proton X. For example, I have all the 4 lines of equal intensity. Let us say this is the chemical shift and then from this to this let us say if this is A, this could be half AM coupling and this could be half AX coupling. Similarly, this side half AM, half AX. If you go to the M spin that will be different one. Like that we can work out and show that all the 4 are

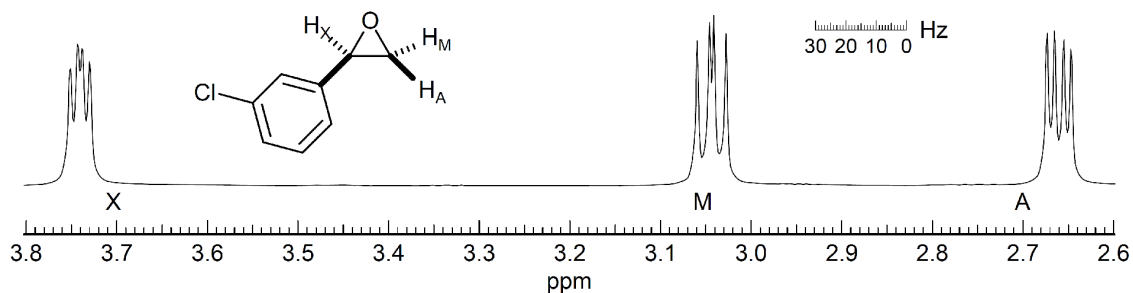
<b>Transition Between states</b>	<b>Spin states</b>		<b>Transition Frequencies</b>
<b>5-4</b>	<b><math>\beta\alpha\alpha</math></b>	<b><math>\beta\alpha\alpha</math></b>	<b><math>-\nu_A + \nu_M + \nu_X</math></b>
<b>7-2</b>	<b><math>\beta\beta\alpha</math></b>	<b><math>\alpha\alpha\beta</math></b>	<b><math>\nu_A + \nu_M - \nu_X</math></b>
<b>6-3</b>	<b><math>\beta\alpha\beta</math></b>	<b><math>\alpha\beta\alpha</math></b>	<b><math>\nu_A - \nu_M + \nu_X</math></b>

allowed. Of course, I also showed you once when I was discussing the selection rule there are 3 possibilities of all the 3 spins can flip at a time. These are called the combination transitions. The 3 combination transitions are allowed here.

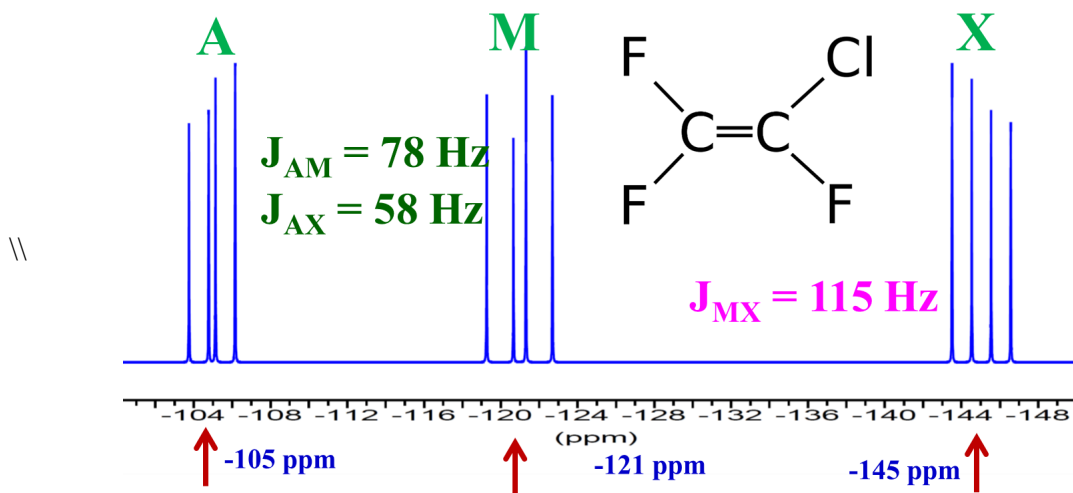
But the combination transitions arrive only at the sum or difference of the chemical shifts. It does not contain J information; and usually they are very very very weak in intensity, and they are seen only in the strongly coupled case. In the weakly coupled case you do not see them. That is the reason why when I took the 3 weakly coupled AMX spin system we got only 12 lines. Only if you go to analyze the ABC case, all the 3 are strongly coupled spins, you will get 15 transitions; including these 3 combination transitions. So, combination transitions will not give J coupling information. And that is what we discussed. This is a simple example of weakly coupled 3 spin case. You see when it is weakly coupled 4 for A, 4 for M and 4 for X, all are of equal intensity. Remember that is why we are going to see very clear spectrum. And this is the center of this, and from the center of the chemical shift of this, one half of this is one coupling, this one is half of another coupling. This is half of other coupling this is half of other coupling. So, from the center you have 2 peaks on the right side, and 2 peaks on the left side, for this, this is a 600 MHz spectrum, very well separated in the 12 lines are of



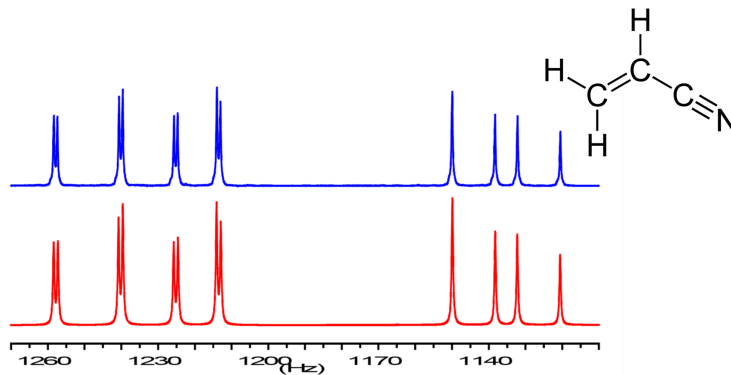
equal intensity. This is a real true example of an AMX case. And you go to the center of this, if you expand it, you get only 4 peaks. Very easy to analyze. I told you the spectrum of weakly coupled spin are very easy to interpret. We can easily extract the couplings and chemical shift information for all the 3. Of course, you can come across a situation you can think of an AMX, but not true AMX, because there will be a minute ABC character will be there. An example like this. Look at the example like this this is.



In principle this, this and this are the 3 protons you can find out very well separated; the chemical shifts are very well separated appears like AMX, because there are no additional peaks like ABC, there are no combination transitions are seen. Here only 12 peaks, but really if you carefully see they are not of equal intensity. That means there is a minute ABC contribution. That is why in principle of course, you can analyze and get the J coupling information and chemical shifts, but if we are hard core NMR spectroscopist we do not accept it, because it is still not AMX. You can analyze by the first order approximation, it is Okay. But you need to still go to higher magnetic field and then make sure all the 4 lines are of equal intensity, so, that you can extract the chemical shifts and the coupling information, and make it weakly coupled. As I have been telling you, a strongly coupled spin will become weakly coupled when you go to higher and higher magnetic field, why? because chemical shift as I told you varies linearly with the magnetic field. If you increase the magnetic field the chemical shift separation keeps on increasing. As a consequence what happens the strongly coupled spin system will become weakly coupled when you go to higher magnetic field. So, for this there is a little sting of a strong coupling character like this. What you are advised to do in case if you want AMX? You have to record the spectrum at a even higher magnetic field; at a higher frequency NMR spectrometer. Look at this one, this is again trifluoro vinyl chloride, a beautiful AMX case, for all practical purposes. This is a fluorine NMR.



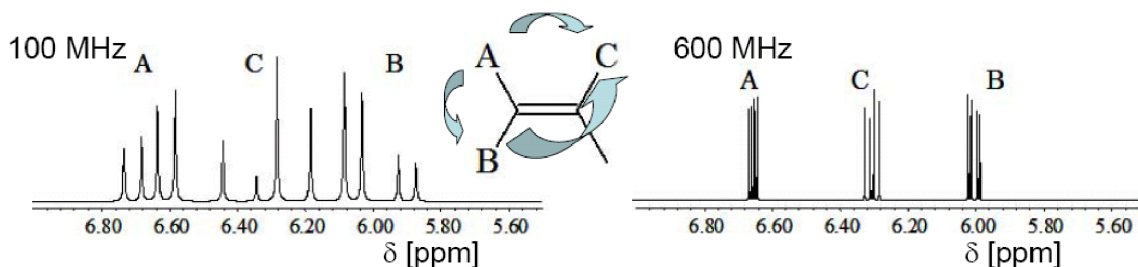
You can see all the 3 lines are of equal intensity. In principle it should be, but there is some sort of a deviation in the intensity. This skewing direction tells you this is coupled to this. This queuing direction tells you this spin is coupled to the one spin which is resonating towards its right. The direction of skewing tells you this spin is coupled to spin which is resonating towards its left, and this is a roof effect. I told you the roof effect becomes stronger and visible more prominently in strongly coupled case. As a consequence I do not consider this as a weakly coupled AMX, it is AMX with sting of ABC character. What you want to do if you want to make it a perfect AMX, remember fluorine was recorded at 56.4 MHz that means, it is a very low frequency spectrometer of 80 MHz n m r spectrometer or so. On the other hand record this fluorine NMR at 400 megahertz then fluorine comes, in the 400 MHz spectrometer at 370 or 380 whatever that frequency. In which case what is going to happen is all the 4 lines I mean all the 4 lines of A, M and X, will become equal intensity. That is the true AMX, you understand. So, true AMX you will get only at higher frequency. This is another example of a molecule at 200 MHz, the spectrum which gave AMX pattern with minute ABC character.



Look at  
are

this one, these 3  
protons and it

looks like there are 4 peaks here, 4 peaks here, and 4 peaks here. What normally the chemist will do, they will take the NMR spectrum of this measure this chemical shift and say I got the chemical shift and J coupling. It is Ok, to report to some extent, but in principle as I told you when this spins are strongly coupled it is not possible to get the individual chemical shifts you can only get the difference in chemical shifts. Individual chemical shifts cannot be obtained. But in this case we can assume for all practical purposes they are weakly coupled and you can get the chemical shift from this one, from the center of this, this one j coupling is from here to here, and another j coupling is here, like this you can extract J coupling for all these things. So, this is way you can analyze this thing. Of course, you can go further and continue this one and see what is going to



happen. I will show you a simple example how the spectrum becomes completely different when you go to higher frequency.

Can you imagine this is a spectrum of a real molecule? There are 3 protons here, with some substitution. Look at this spectrum these are 3 spins. We have written a b and c, but I do not know which is which is a, which is b and which is c. We cannot mention it easily, but for just for the sake of explanation it is written like this and look at the number of peaks here and their intensity pattern. You cannot extract this and analyze from the center of the this is a this is a, m and x like that. You cannot do that. You have to simulate it you have to do the computer analysis, get the real frequency of the transitions and the intensities. Only then you get the chemical shifts and J coupling information. Otherwise straight forward first order analysis is not possible that is what I have been telling you.

So, in strongly coupled spins you cannot analyze the spectrum in easy way. This is not possible. This is called second order analysis; where you need to do computer simulations for all the frequencies, and all the transitions intensities. Look at this one, 600 MHz spectrum, very well separated peaks. Looks like ABC becomes AMX here. Strictly speaking if I give you the spectrum and say is it AMX your answer should be no, because look at this intensity they are not equal. But for all practical purposes compared to this, it is easy to analyze and you can assume it is a AMX case. There is no problem although there is minute ABC character present in this. This is what ABC at 100 MHz became AMX at 600 MHz. Here this is 600 megahertz. if you really want to get a pure AMX instead of 600 you have to go to 900 megahertz or 1 gigahertz, then you can see all of them with equal intensity, really a pure AMX with all equal intensity. So, strongly coupled becomes weakly coupled at higher field, this is what I just wanted to tell you about the Pople nomenclature and coupled spin system. And I took the example of the 3 spin case here took AMX. But if you take ABC, what will happen? you will not get 12 peaks you will get 15 peaks. There is no way you can analyze it in a straightforward way.

What happens if you take A<sub>3</sub>, all the 3 are chemically equivalent, there is no chemical shift difference at all. All of them appear at the same frequency. There is no difference in chemical shift, then it is A<sub>3</sub> with the coupling we present or not. In the A<sub>3</sub> coupled spin system it can be present it need not be present, does not matter. But it always gives a single peak ABC gives 15, AMX gives 12 transitions, AB<sub>2</sub> give 9 transitions. So, depending upon how the spins are coupled whether they are strongly coupled or weakly coupled, you can get lot of different types of spectra. And lot of information can be obtained by analysis, except for AMX no other strongly coupled cannot be analyzed in a straight forward manner. So, this is what I just want to tell you about the way we have to

analyze the spin system. Of course, lot more thing can be done. even in 3 spins there are so many nomenclatures I gave you. If you have to analyze each of them, they can be analyzed write down the spin system, write down the Hamiltonian, diagonalize the Hamiltonian and then get the Eigen values and frequencies. And then you can do simulation and get all the information. It is a laborious work it cannot be done so easily. But I do not want to discuss all those things, but I just wanted to give you an idea. You need to use the proper nomenclature to analyze the spectra.

So, this is what I wanted to tell you about the Pople nomenclature. And next we will go to the interpretation, the real interpretation of the one dimensional NMR spectra, 2D NMR spectra etcetera later. First we will start with the 1D NMR spectral analysis and today what we have covered already. So, from the 2 spins I said we give maximum of 4 transitions. If you have a 3 coupled spin system we can have maximum of 15. If you have 4 coupled spin system, 56 transitions because the number of transitions are given by the formula  $2^N C_{N-1}$ . N is the number of coupled spins, put the value of N and calculate the number of transitions. As the number of spins become more and more go to 6 spins 792 transitions, if you go to 7 spin 3003 transitions you will get. So, it is very very complex spectrum, but most of them are redundant. We do not require that many frequencies to get the spectral information and then of course, I showed you an example of a 3 spin case AMX, how the 4 transitions for A, M and X are obtained. Just by looking at the energy level diagram write down and applying the selection rule. Of course, you can calculate the Eigen values, Eigen frequencies and get the correct frequencies. And the intensity will be exactly 1 is to 1 is to 1 is to 1, for each coupled spin system in the AMX if you will get 12 transitions. But it is not the case with a strongly coupled case, that is what I just wanted to tell you. I will stop here, we will come back and continue with other things in the next class, the analysis of the proton NMR spectrum. Thank you.