

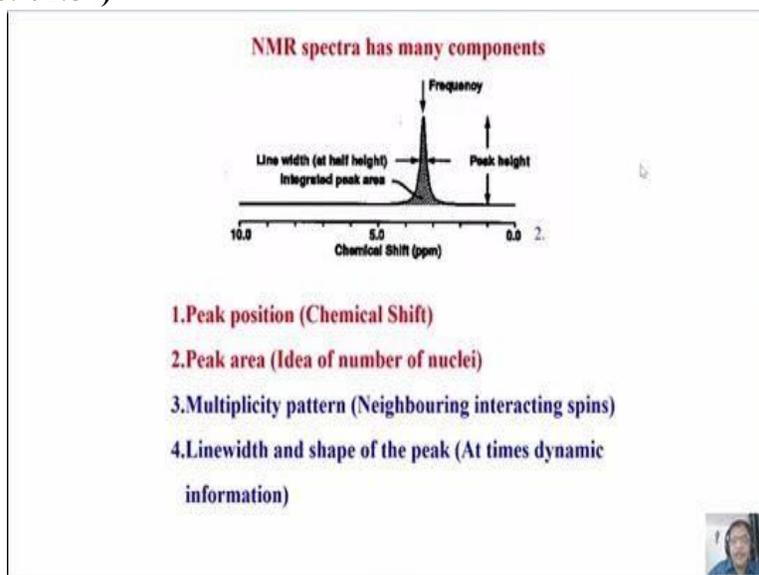
One and Two Dimensional NMR Spectroscopy for Chemists
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Lecture - 18
Scalar Couplings

Welcome back. In the last couple of lectures, we discussed about chemical shift, one of the most important NMR parameters, which arises because of internal interactions, that was the interaction of the nuclear spin with the magnetic field, which is because of the electronic environment surrounding it, which shields the nucleus, and we understood a lot about chemical shift, what happens to it with the magnetic field? And what is the difference between the ppm and chemical shift scale, and various things, and the factor that influences chemical shifts, everything we understood. I hope you are all with me. Today, I am going to discuss another very interesting NMR parameter, which is responsible for understanding the multiplicity of the NMR signals, which tells you what is next nearest neighbor and subsequent neighbors, like that.

And this helps in assigning and getting the structural information, conformational information of the molecules. It is one of the very, very important things to find out. If I am looking at a proton, I want to know what is the functional group sitting next to it, or covalently bonded to it. That type of information, very easily we can derive, by understanding scalar couplings.

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Before that, let me tell you the NMR spectrum has many, many components. First of all, if I look at the NMR spectrum like this, which I said how to get the resonance in the couple of lectures before. Look at this one, this is the shape of a peak. There are several information which is contained in this first thing, the position at the peak, that is what we have been discussing in the last couple of classes, that is what is called chemical shift with respect to some reference which you use in a particular nucleus observation, what is the position.

For example, in proton with respect to tetramethyl silane, what is the chemical shift position in frequency or ppm of a particular peak. So peak position is important. Second area of the peak, I told you remember, the area of peak gives you the number of protons present, relative to other peaks. I have to have some reference, some peak, if I know what are the number of protons present in that, with respect to that, relatively with the peak height, I can find out, I can tell you the number of protons present in that. For example, if to the CH₃ group, if I know we have the C-H group, I know C-H group comes because of single proton, then related to that I will say this intensity must be 3, and this should have 3 protons. Like that, the peak area tells you, identify the number of nuclei, number of spins or number of protons, which are responsible for this.

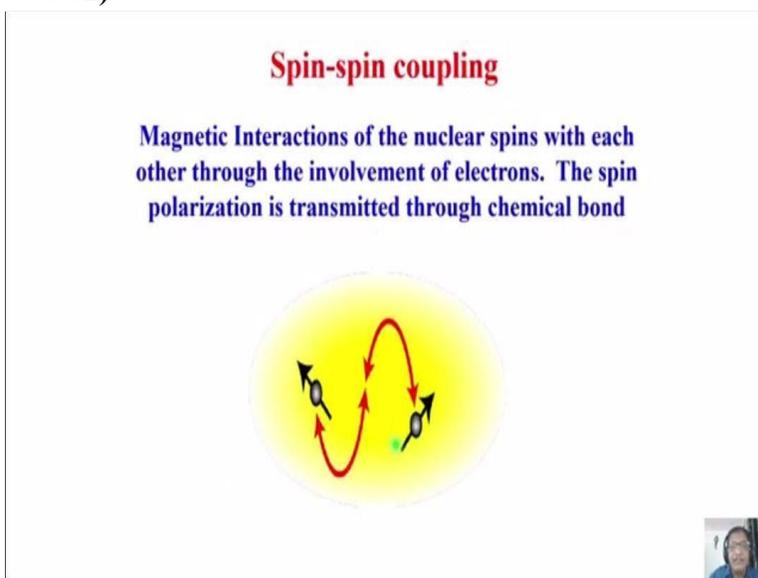
And, another interesting thing what we have to discuss from today's class is the multiplicity pattern. This peak assuming there are no other neighbors which are interacting with it, it is going to be a single peak. Assuming I am looking for a proton in a molecule, or hydrogen where it is resonating, if I look for the chemical shift of it, if all the neighbors are far away, and there is no interaction of other protons, or any other NMR active nuclei, with this particular proton of interest, it will be a single peak. If it starts interacting, then this peak starts giving rise to multiplicity, it starts undergoing splitting and we get multiplicity pattern.

The multiplicity pattern can be different types, various types, it could be 2 lines of equal intensity or it could be 3 lines of equal intensity, it could with 3 lines of different intensity like 1 : 2 : 1, varieties of things happen. So that multiplicity pattern tells me what are the neighboring interacting spins. What are they? and how this is split because of them. Second, is line width and shape of the peak. The shape of the peak and line width also gives me, sometimes dynamic information.

If, let us say I have 2 peaks, assuming that I have taken NMR spectrum, one peak is very, very sharp, other peak related to that is very, very broad. This has an information content, it tells me why this peak is broad, it is undergoing fast relaxation or it may be undergoing some dynamics, it may be undergoing exchange, some dynamics is going on with this proton. As a consequence, it is going to be relatively very broad compared to the peak. So, it gives me information about the dynamics of the molecule. So, NMR peak has several information.

So, now we have to understand, first we understood the peak position in the last couple of classes, that is chemical shift where it comes with respect your reference. Now, we also understood the peak area, which tells us the number of protons, which are responsible for that peak. Today, we will understand multiplicity pattern, how the neighborings interact spin with the proton of my interest, and how the multiplicity arises. Of course, as a consequence, we also understand later about the dynamics, how the line width and shape of the peak gets affected. OK.

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With this information, let us start discussing about spin-spin coupling. As I said, remember, except quadrupolar interaction, all are magnetic interaction. It is the magnetic interaction of the 2 nuclear spins, let us say, this is one nuclear spin, this another nuclear spin. There is a magnetic interaction between these 2 with the involvement of bonding electrons. Remember there must be a covalent bond between these 2. With the involvement of a bonding electron, the nuclear spin here transfers its polarization or magnetization to this or this can interact with this.

So, as a consequence the polarization is transmitted through covalent bond. For that the medium is bonding electrons, that is necessary. Remember, this nucleus spin can see this one through covalent bond.

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J-coupling mechanism

Fermi contact term mechanism is the dominant one for all couplings involving hydrogen. The interaction between two spins arise because of bonding electrons.

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Take C-H bond, connected by a single sigma bond, having two electrons

The magnetic moment of hydrogen can be either parallel or antiparallel to the magnetic field

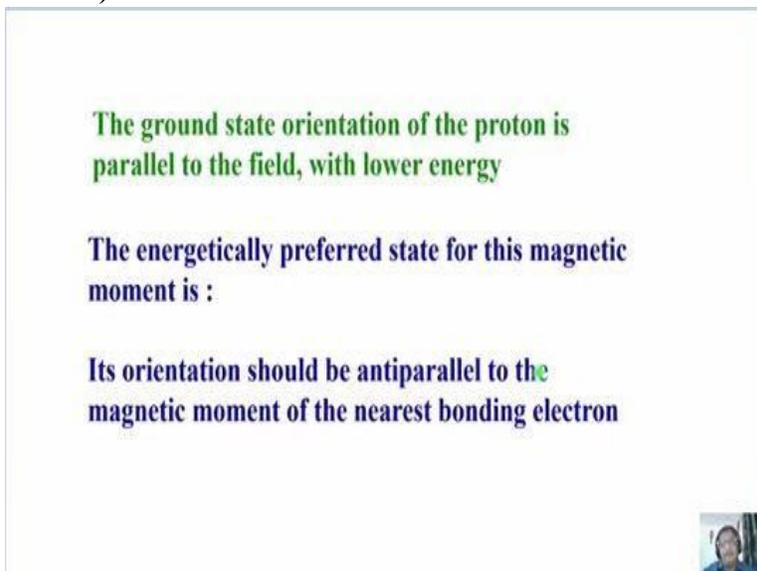


If that is the idea, what is the mechanism, how this nuclear spin, one nuclear spin sees the other nuclear spin. How do they interact? One of the dominant interaction mechanism, is what is called Fermi contact interaction. Fermi interaction. This arises because of bonding electrons. Remember, the Fermi interaction is there, that is very important and we will start by taking an example of a 1 single CH bond. Here carbon 13 is an interacting spin. carbon 13 has a spin. It has spin half, proton has spin half. I take this CH bond. So, both spins are having spin half, both are tiny magnets, I said. They will interact. The nucleus of carbon, the nuclear spin of carbon can interact with nuclear spin of hydrogen. In other words, the magnetic moment of this carbon can interact with the magnetic moment of this hydrogen or this proton. Now, it must be connected by a sigma bond with having two electrons, that is what C-H bond we are considering. We consider C-H bond. It is connected by a single sigma bond.

An I am isolated C-H bond I am taking, forget about what other things that we attach to this carbon spin, for this proton, I am not bothered. Just for understanding purpose, I am taking a C-H bond. It has a single sigma bond with 2 electrons, it is well known in chemistry. Now we will start looking at one of the nuclei either carbon 13 or proton, does not matter. You can take anything you want. Let us consider I will take the hydrogen atom.

Now, moment I put the nuclei spin in a magnetic field, what are the possible orientations? The magnetic moment of this hydrogen has 2 possible orientations, because it is spin half. As a consequence, there are 2 possible orientations for this magnetic moment, one in the direction of field, and the other in the direction opposite to that of the field. Please understand, now, the magnetic moment of hydrogen has 2 possible orientations, in the magnetic field. With that idea, let us start, to go further.

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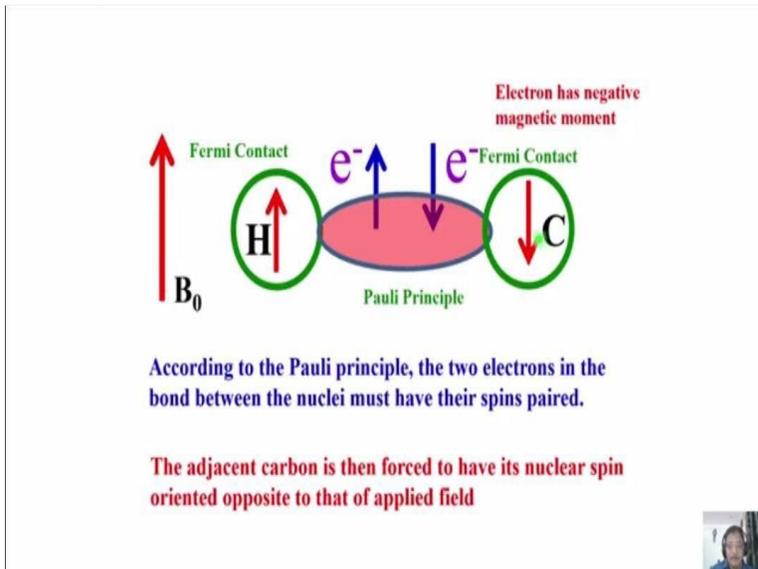
Let us take the ground state orientation of the proton. What is the ground state orientation, which is alpha first state, which is parallel to the field, lower energy. We will consider alpha state, which has orientation of the proton parallel to the field, which has low energy. Now what is the energetically preferred state for this magnetic moment? Now I am considering nuclear spin, proton coupled to carbon with a sigma bond, where there are 2 electrons.

The energetically preferred state for this magnetic moment is, the orientation of this should be antiparallel to the magnetic moment of the nearest bonding electron. Please understand this statement. The orientation of this proton, now I am considering proton, with the ground state of the proton with the orientation parallel to the field, that is the lowest energy configuration I said. This is lowest energy option. The spins that orient parallel to the field has the lowest energy.

That is what we have been discussing from the day one, but for this to be energetically in a preferred state, the electron which is attached to this which is forming a bond must be

antiparallel to this, if this is the orientation of the magnetic moment of proton, the electron magnetic moment should be antiparallel to this. This is the preferred orientation, This is the minimum energy configuration for this, that should be there.

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Now, let us see the drawing, how it orients diagrammatically we will try to understand. I have done a crude diagram myself. Do not worry about it. My drawing may not be very good I not a very good artist, does not matter, look at this proton spin. I have taken it to be in the direction parallel to the magnetic field, lowest energy. Only one component of this magnetic moment which is in the direction of the field, if I take. Now, the Fermi contact tells me, because of that this electron has to be antiparallel to this, that is the preferred energy state.

But the question is why did the right parallel to this? remember, even though I have written diagrammatically like this, this is lowest energy for this because the electron has a negative magnetic moment. Please understand. Electron has a negative magnetic moment. As a consequence, even though those these 2 are parallel, that is minimum energy. It is as good as telling, this proton, this electron is antiparallel in orientation to this proton magnetic moment. Please remember this point. That is why diagrammatically I have shown this to be in parallel to this magnetic moment, because electron has a negative magnetic moment, so far so good. Now, what is the next one? Look at the other bonding electron. There are 2 electrons in the sigma bond. Now, you will understand the Pauli principle. What does the Pauli principle say? these 2

electrons should be paired. The 2 electrons, between these 2, must be paired. The bonding electrons must be paired.

So when this is in the direction parallel to the field, then this must be opposite to this electron. I know, because of this orientation parallel to the field, I know what is the orientation of this electron, and as a consequence I know orientation of this bonding electron. Now, when this is like this, this must be opposite to this electron. But I represented in the same orientation again because this has a negative magnetic moment.

So, the configuration can be easily understood in a simple diagram. I consider the parallel orientation of magnetic moment, lowest energy possible orientation of this nuclear spin is in a direction parallel to the field, this orients electron opposite it, this electron gets paired with another electron which is in the sigma bond, with respect to this, and this electron orients this proton opposite to this. I am sorry, this carbon nucleus opposite to this.

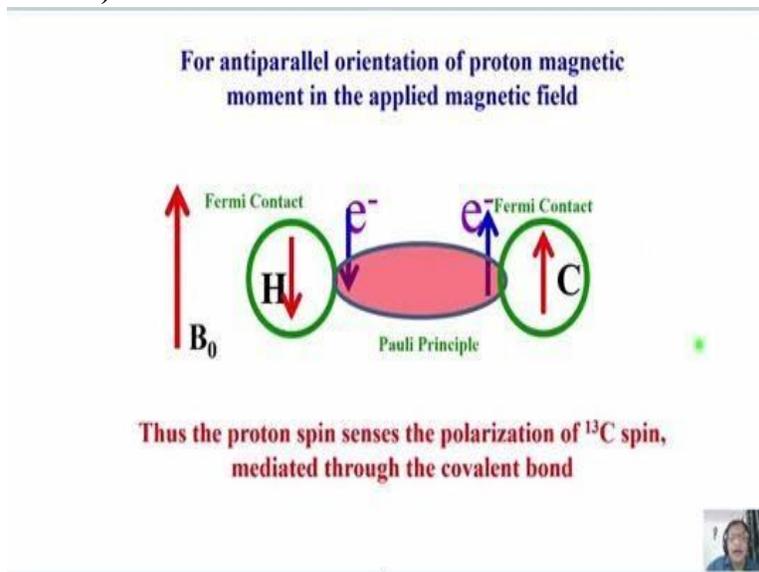
So, now I understood the orientations of proton and carbon, what does it do, the adjacent carbon now, because of this type of mechanism, first Fermi contact, then Pauli principle pairing up, then again Fermi contact, and these interactions will force the neighboring carbon to have its spin oriented opposite to this field. Please understand the concept now. I took initially the proton to be in the direction of the field.

When I went to Fermi contact, first Fermi contact, then Pauli principle of electrons getting paired, again this electron can have Fermi contact with this carbon. Finally, because of this, this proton ensures or forces this carbon direction oriented opposite to this field. Now, let us look at the orientation of 2 nuclear spins, proton and carbon, they are oriented opposite to each other, by this mechanism. So, I started with the parallel orientation of proton spin with respect to field and ended up getting carbon orienting opposite to the field by a single sigma bond.

Remember, this is a consequence, why does it happen? Because that is the favored configuration. Now, you may ask me a question, fine. This due to the parallel orientation. There are 2

orientations for a proton spin. You took the parallel orientation, what happens if you take the opposite one? that question you can ask, true.

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We can also work out the same way. Now you take this as a negative orientation. Correspondingly, this electron gets oriented opposite because it has a negative magnetic moment, I am showing you the same direction, this gets paired with the bonding electron, this forces the carbon spin to align in a direction parallel, you understand. So, now, whether you take parallel orientation of the new magnetic moment of proton or antiparallel orientation with respect to the field, it always ensures the carbon spin orients in the direction opposite to its magnetic moment.

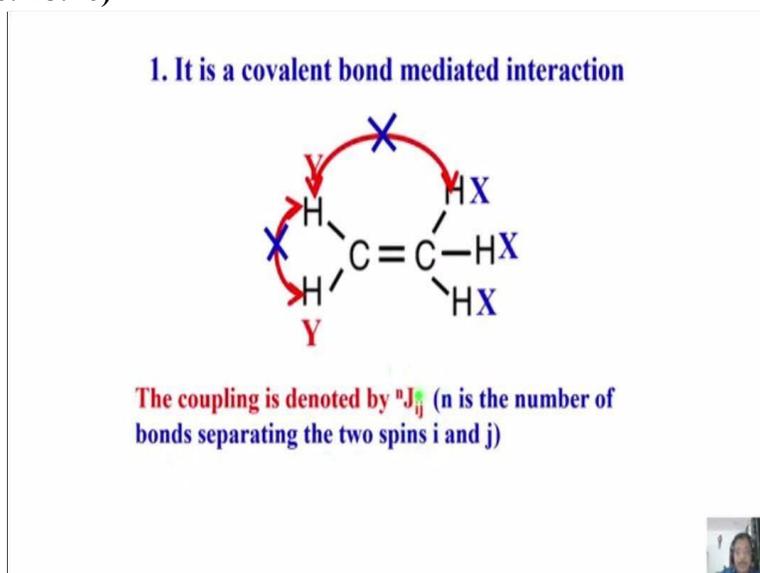
And with this step, what I can say, with this type of interactions, I am telling carbon 13 spin sees the polarization of protons. It senses this polarization, or in other words, the proton spin senses the polarization of carbon, either way is correct. Please remember, do not get confused. What I said, whatever be the direction of orientation the magnetic moment of proton state, it forces the carbon adjacent to it, bonded by a single sigma bond, in a direction opposite to it.

Nevertheless, the simple concept you understand, the protons spin, senses is the polarization of the carbon spin, which is mediated through covalent bond. This is what is called scalar coupling. An interaction between 2 nuclei, magnetic nuclei which are NMR active, through covalent bond, is called spin-spin coupling, or J coupling or covalent bond mediated coupling. All these are the terminologies. please remember, this is called covalent bond mediated J coupling.

Now with this you can understand a lot about this coupling, we will go slowly one by one, many things are there for us to understand before I go. I will give you some salient points of scalar coupling, please remember, that these are very important points. I have compiled all those things for you people to understand very clearly, please remember these are points, like a bullet points I am giving you. Take a note of this.

Remember each and every point is very useful and we will discuss these things later. Today and next to 1 or 2 classes or 2 or 3 classes, we will be talking only about scalar couplings, a lot more of these things we will discuss. So I start listing one by one.

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First, just now I discussed. It is a covalent bond mediated interaction. It always a spin polarization of one of the protons, that will go to the other spin which is interacting with this, only through covalent bond. For example, I have a CH₂ group and CH₃ group do not go into the details of the molecular structure, as whether C valence s matching or not, all those things I am not worried about that, I just wanted to show you something just to see.

Now according to the statement of mine, what is the J coupling? Let us take this proton, this proton can interact with this proton through this bond. It comes to proton to carbon. Let me show you the polarization of this proton is sensed by this carbon, this is further sensed this carbon and

this polarization is further sensed by this proton. See this proton interacts with this. Because of that, both Fermi contact, Pauli principle and then again Fermi contact, like that it keeps on going.

So, the magnetization or polarization of this proton is transferred to this, from this carbon to this through bond and this carbon to this proton through bond. So, it is the covalent bond mediated interaction like this. You may ask me a question, what about this proton and this proton, they are nearby in space. No, there is no direct transfer of magnetization through space. This covalent bond mediated interaction, scalar coupling, has to be only through bonds, covalent bonds.

If we choose through there are examples, 1 or 2, I will come to that later. There are deviations from this, but majority or, or all the times, the rule is basic rule, remember, it is mediated through covalent bond. This is the first point, and this is also not allowed. Now, the coupling is always denoted by ${}^nJ_{ij}$, where n is the number of bonds separating 2 spins, i and j are the two interacting spins. Now we will go back to this molecule, this example, this proton is coupled to this, how many bonds are there? 1, 2 and 3. So this proton and this proton are separated by 3 bonds.

And if I call this as proton x , and this as y , so what is my nomenclature? ${}^3J_{xy}$. So these 2 protons are separated by 3 bonds and the interaction is between this spin and this spin. So i and j refer to the interacting spins, n tells you the number of bonds they are separated, sequentially, you can't take this proton and some other proton. So, it has to be sequentially get separated. So, you cannot draw a line here and say it separated one bond, No. You have to go through chemical bond. So now you know what is the nomenclature we use for measuring the coupling strength between 2 interacting spins, it is ${}^nJ_{ij}$, n is the number of bonds separating the 2 spins, i and j .

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2. J couplings depends on the electron charge density at the nucleus and are not averaged in solution state

Hence it does not depend on the orientation of internuclear vector

That is why it is called the scalar coupling

3. The strength of the interaction is few Hertz to few tens of Hertz



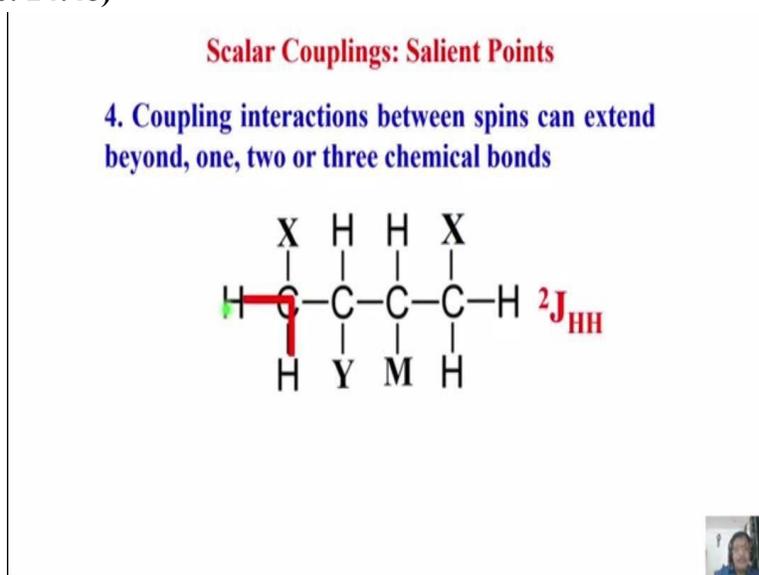
Now, another thing, J couplings depends on the electron charge density at the nucleus and are not averaged in solution state. Very interesting thing, J coupling is not averaged out in the solution state. Please remember, in 1 or 2 class, first or second class when I was discussing with you, I did say that dipolar coupling is direction dependent, it is orientation dependent. I said that gets averaged out in solution, is the motional averaging in the solution, it vanishes.

That is what I said. But I also said J coupling do not vanish, this is the reason it depends on the electrons charge density and does not average out in the solutions state, it does not depend on the orientation of internuclear vector, unlike dipolar coupling. So, the J coupling has no direction dependence. That is why it is called scalar coupling. If it has a orientation dependence you can call it a vector. So it is not direction dependent. It has no direction, it is simply a number, that why it is called a scalar coupling.

Another salient point, point number 3, the strength of interaction is few hertz to few 10s of hertz. Let us say, the 2 protons are J coupled. How do you express its interaction strength, it is always expressed in hertz. J is always express in hertz, remember chemical shifts is expressed in ppm, delta, but J is always expressed in hertz. So, it can be a few hertz, 10 hertz, 5 hertz. 0 hertz or too close to 0, we may be from 0.1 hertz to a very large value, in heteronuclear case it can be very large also.

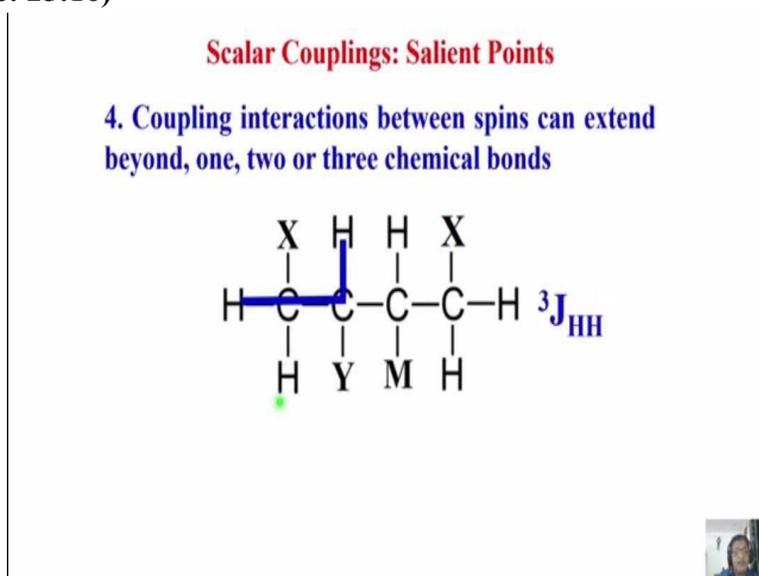
So, it depends upon the coupling strength, whether it is homonuclear heteronuclear. If the coupling is between like spins, i.e. homonuclear spins, there are ways we can say what are the couplings, whether it is 1 bond 2 bond 3 bond, like that. Similarly, if they are heteronuclei also we know. Remember one thing, the strength of interaction is always from few hertz to 10s of hertz. It can be 1 hertz 2 hertz to several 10s of hertz.

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Point number 4, coupling interaction between the spins can extend beyond 1 2 or 3 bonds. It is not always 1 bond, I just now showed. It can extend up to n number of bonds. For example, in this case, it is separated by 2 bonds, with our nomenclature, it is called ${}^2J_{\text{HH}}$, remember.

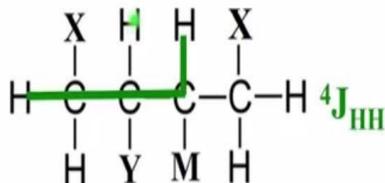
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Scalar Couplings: Salient Points

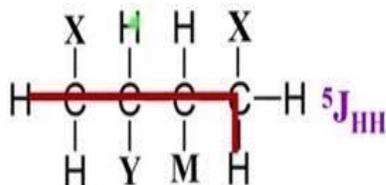
4. Coupling interactions between spins can extend beyond, one, two or three chemical bonds



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Scalar Couplings: Salient Points

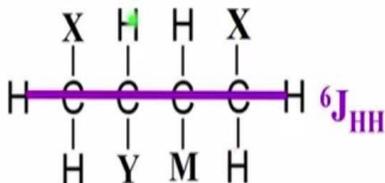
4. Coupling interactions between spins can extend beyond, one, two or three chemical bonds



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Scalar Couplings: Salient Points

4. Coupling interactions between spins can extend beyond, one, two or three chemical bonds

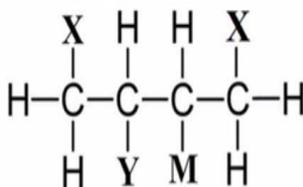


Now, what is this, it is separated by 3 bonds 1 2 and 3, it is ${}^3J_{HH}$, what about this? ${}^4J_{HH}$ this is ${}^5J_{HH}$, this is ${}^6J_{HH}$. So, it can extend beyond 1 2 or 3 chemical bonds. Of course, the interaction strength decreases, I tell you later as we go. The strength of interaction is more when it is 1 bond, or 2 bonds, and in the same order it decreases. 1 bond is larger than 2 bond, it is larger than 3 bond, then 4 bond, 5 bond, like that. In always there are some deviations and exceptions in NMR, that we will discuss later. But this is the important point, the coupling interaction between spins can extend beyond 1 2 or 3 chemical bonds.

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Scalar Couplings: Salient Points

4. Coupling interactions between spins can extend beyond, one, two or three chemical bonds



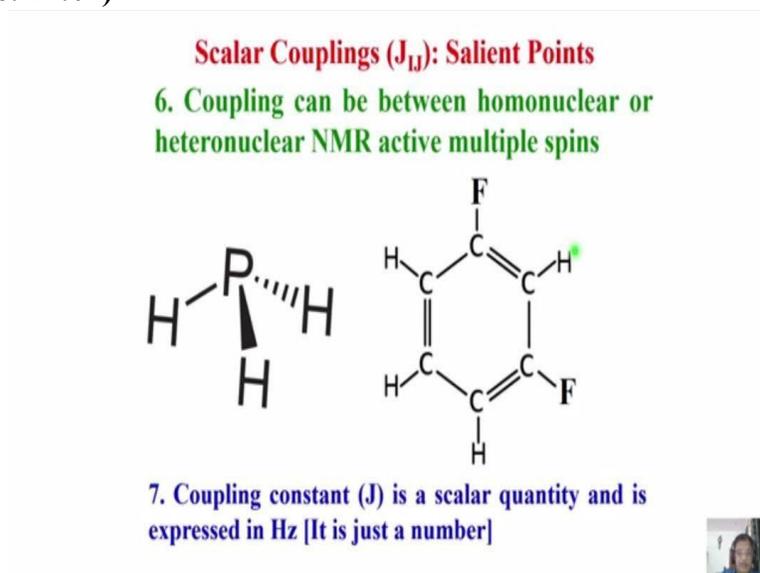
5. The value of coupling can be positive, negative or zero

Another point, the value of coupling can be positive, negative or 0. If I say that 1 bond or 2 bond interaction between this proton and this proton is 10 hertz, it is all expressed in hertz, I said

coupling strength is an hertz, if it is 10 hertz what is 10, is it + 10 or - 10? the sign is important, I am telling you only the magnitude is 10, but it also has sign. The J coupling has the sign. So, the coupling can be positive or negative, but it can be 0 also. So, there is a J coupling, but J coupling value will be 0.

See, for example, this, this and this, if I take, this coupling, the 3 bond coupling may be close to 0, and this may be larger, sometimes 3 bond coupling may be 0 but 4 bond coupling may exist. We do not know, it can happen. So what it means the value of coupling can be positive, negative or it can be 0 all are possible.

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Point number 6 coupling can be between homonuclear heteronuclear NMR active multiple spins. very important point the coupling is not always between homonuclear, it can be between homonuclear spins and heteronuclear spins. For example look at this molecule phosphorus and proton, there can be coupling. This is 1 bond coupling. That is allowed, though they are not like spins, unlike spins, they are heteronuclear spins, between proton and phosphorus there is a coupling, and this is also possible. And look at this molecule, I am looking at fluorine intentionally I have put 2 fluorines here.

Now, this coupling can be there, homonuclear, this heteronuclear coupling can be there, homonuclear coupling is between 2 protons, heteronuclear between proton and fluorine is there, heteronuclear coupling between carbon and proton is also there, homonuclear coupling between

2 carbons can be there and at heteronuclear coupling between carbon and fluorine is there and homonuclear coupling between fluorine and fluorine is also there, and heteronuclear coupling between fluorine and proton is also there. Imagine I have got 3 nuclei here, I can get all possible homonuclear and heteronuclear couplings possible. There is no rule that it should couple only to homonuclear spins, it should couple only heteronuclear spins. every coupling is possible, so, long as they are NMR active nuclear spins present in your molecule, there can be coupling among homonuclear spins and also heteronuclear spins of varied strengths. You understood now,

There are so many couplings here, homo between protons, hetero between proton and carbon, homo between carbons, hetero between proton fluorine, and homo between fluorine and fluorine. All these things are possible, and the coupling constant is a scalar quantity and is expressed number. It is in hertz, it is a number, I will say coupling between 1 bond, or 2 bond coupling, etc. maybe 5 hertz 10 hertz. I express it in terms of number, and its unit is hertz. it is just a number.

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Scalar Couplings: Salient Points

8. The magnitude of the spin-spin coupling between the coupled spins decrease with the increase in the number of bonds. Usual trend, but can be exceptions

$${}^1J_{\text{HH}} > {}^2J_{\text{HH}} > {}^3J_{\text{HH}} > {}^4J_{\text{HH}}$$

9. The coupling constants are independent of the applied magnetic field.

10. The splitting patterns are independent of the signs of the coupling constants



Scalar coupling point number 8, the magnitude of the spin-spin coupling between the coupled spins decrease with increasing number of bonds. Very interesting point. Remember, as the number of bonds sequentially keeps on increasing, take a molecule now, number of bonds keeps on sequentially increasing. The coupling strength keeps on decreasing. Take for example 1 bond proton, proton coupling. This is larger than 2 bond proton, proton coupling, this is even larger than this, one 3 bond. 3 bond coupling is larger than 4 bond coupling. This is a usual trend.

Usual trend is, the coupling strength decreases with the increase in the number of bonds. But there can be exception, there are always some 1 or 2 deviations and exceptions in NMR. We will discuss that later.

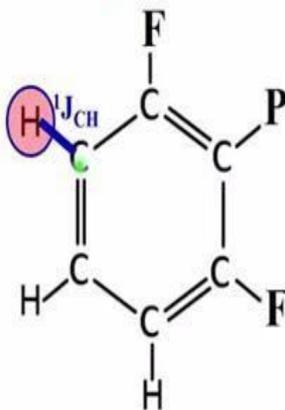
Point number 9 the coupling constants are independent of the applied magnetic field. Very interesting point. I measure the coupling constant between 2 protons let us say, or between proton and carbon at 400 megahertz. It is said at 400 megahertz coupling between 2 protons is 20 hertz. Go and measure the coupling at 800 megahertz, again 20 hertz it would not change. It is field independent. Remember, in chemical shift, what we were telling, it is field dependent. See the beauty of NMR, chemical shift is dependent on field, it is linearly changes. Whereas couplings are independent of the magnetic field. IN whatever the spectrometer you measure, the coupling will not change.

Point number 10, the splitting patterns are independent of the sign of the coupling.

Understand, if I say because of this, I like to explain what is splitting everything when you go ahead further, the splitting pattern, if I say there are 2 peaks coming here because of J coupling, Let us a positive J coupling, I change and make it negative. It simply changes like this, you will not be knowing whether it is positive or negative. As far as we are concerned spectrum remains unaltered. It looks identical whether it is positive sign or negative sign. So, one dimensional spectrum will not discriminate the coupling, whether it is positive or negative.

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11. One spin can simultaneously experience couplings with many other chemically inequivalent spins of varied strengths



Another thing, important point one spin can simultaneously experience coupling with many other chemical inequivalent spins of varied strengths. Imagine I have consider 1 proton or 1 fluorine, 1 atom here, it can be simultaneously experience couplings with all other spins. Not that when this proton has a coupling with this, then it cannot have coupling with others, no its not allowed. Every 1 proton or 1 spin can simultaneously experience coupling with others, with all other spins. So, take for example, now, proton, this proton, this can have a coupling with this carbon.

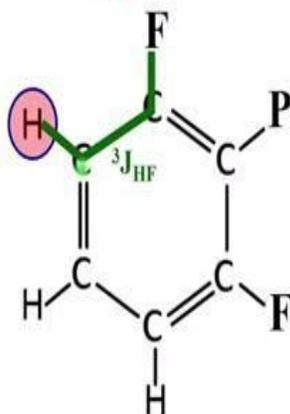
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11. One spin can simultaneously experience couplings with many other chemically inequivalent spins of varied strengths



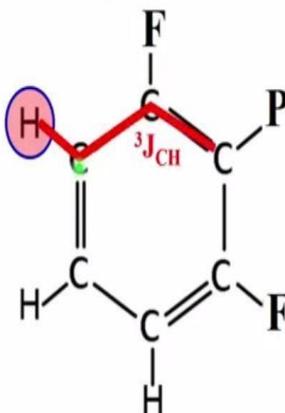
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11. One spin can simultaneously experience couplings with many other chemically inequivalent spins of varied strengths



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11. One spin can simultaneously experience couplings with many other chemically inequivalent spins of varied strengths



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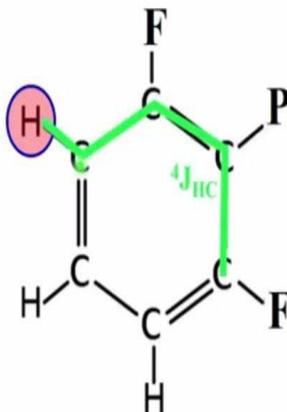
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This can also have coupling with this carbon 2 bond coupling, it can have a 3 bond coupling with fluorine, 4 bond coupling with this carbon, 1 2 3 4 bond coupling with this phosphorus, 4 bond coupling with this carbon, 5 bond coupling with this fluorine, 3 bond coupling with this proton and 4 bond coupling with this carbon. And 4 bond coupling with this proton.

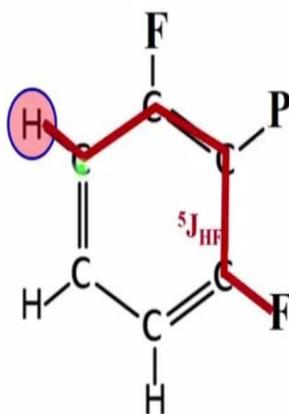
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11. One spin can simultaneously experience couplings with many other chemically inequivalent spins of varied strengths



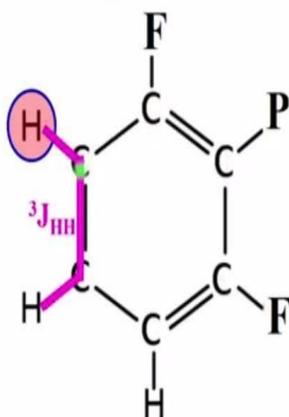
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11. One spin can simultaneously experience couplings with many other chemically inequivalent spins of varied strengths



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11. One spin can simultaneously experience couplings with many other chemically inequivalent spins of varied strengths



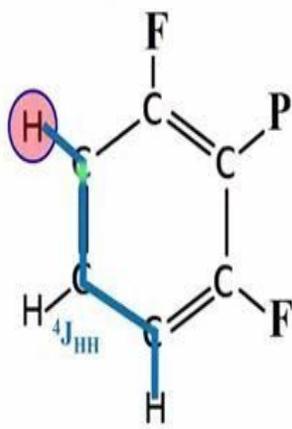
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11. One spin can simultaneously experience couplings with many other chemically inequivalent spins of varied strengths



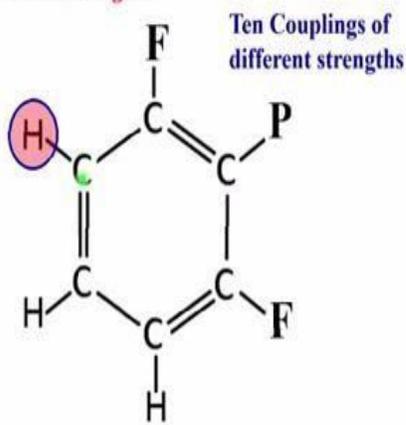
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11. One spin can simultaneously experience couplings with many other chemically inequivalent spins of varied strengths



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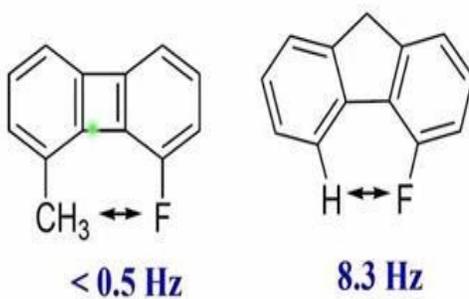
11. One spin can simultaneously experience couplings with many other chemically inequivalent spins of varied strengths



See this proton alone if you have counted, you would have got 10 different couplings, assuming everything is coupled. Assuming all nuclei are coupled to this proton, you can expect 10 different couplings in this. I will again show you one by one, remember, 1 bond, 2 bond, 3 bonds 4 bond, 4 bond with this H, and then 4 bond, 5 bond, these 3 bond, this one, this one, 10 couplings you can get. Maybe I would have missed 1 or 2 if I carefully see. But remember, what my idea was to tell you is that, any one spin can simultaneously experience coupling with many other chemically inequivalent spins.

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In rare cases, "through space" couplings are possible if one atom has lone pair electrons and the two nuclei are in van der Waals contact

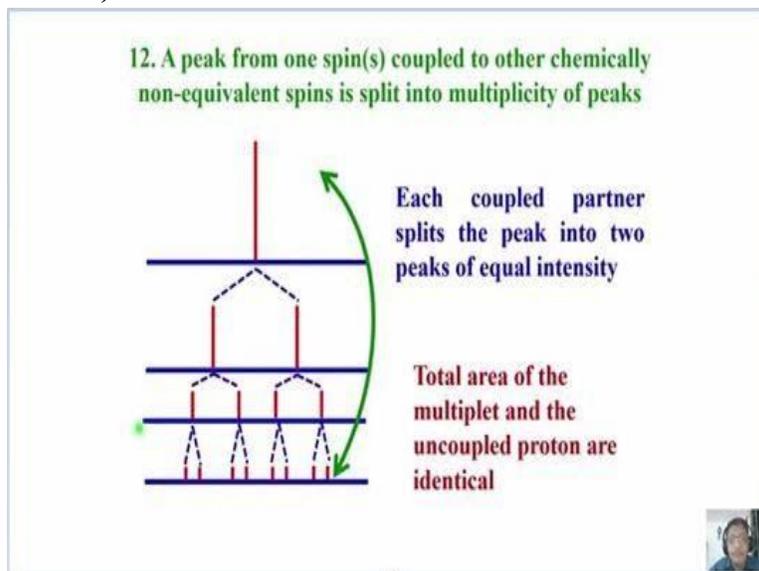


It is not co-valent bond mediated

In rare cases, very, very rare cases, so far I was telling you, covalent bond is a must to see the coupling, but in rare cases, you can get through space coupling like this without going through

the covalent bond, that is example 2 cases like this, where 1 atom has lone pair of electrons or nuclei are within van der Waals contact. Very rarely you can see such type of couplings, Do not worry, that is an exception.

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Point number 12 a peak from 1 spin coupled to other chemically non-equivalent spins is split into multiplicity of peaks. Let us say I have 1 peak from a spin, it is coupled to another nuclear spin is splits into 2. But what happens to its intensity? it comes down to 50 : 50. If it is coupled to another proton, the intensity further again comes down, coupled to another one, again intensity comes down. But each time, each line starts splitting into two two lines. It is like a family tree, like a fiction reaction, 1 becomes 2, 2 becomes 4, 4 becomes 8.

But one important point, you must remember, the total intensity of this peak before splitting and if we take the intensity of all these 8 peaks, it remains the same. The total area of multiplet and uncoupled proton are identical. There is no difference at all, hope you get my point. Very interesting, you must remember this thing. A peak from one spin coupled to other chemically inequivalent spins split into multiplicity. But finally, the area of the uncoupled proton or the number of peaks which has been split into remains same.

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Scalar Couplings: Salient Points

13. Multiplicity of the peaks among groups of chemically equivalent spins is given by $2nI+1$ (weakly coupled spins)

14. For coupling among equivalent spins, the relative intensities within a multiplet are given by the coefficients of the binomial expansion / Pascal triangle



And few are the salient points. The multiplicity of peaks among groups of chemically equivalent spins is given by $2nI + 1$ formula. I will explain to you when I go further. For coupling among equivalent spins, the relative intensities within a multiplet are given by the coefficients of the binomial expansion, called the Pascal triangle. I will come to that later. This point again, I will come back. I will discuss more about these points in the next class, because I cannot take too much of time, because we have been allotted a particular amount of time, within that I have to discuss and then if it is excess, I have come back in the next class. So, you understand basically in this class, I was trying to tell you, bringing another interaction parameter called J coupling, where I told you the mechanism of J coupling, the way it is happening, and some of the salient points, I gave you. These are the points to remember, you will understand more about it later, The salient points, about 13 to 14 points about J coupling, I introduced to you. So we will come back and discuss more about it tomorrow.