

Advance Analytical Course
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Lecture No. # 34

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Two Energy States

The magnetic fields of the spinning nuclei will align either *with* the external field, or *against* the field.

A photon with the right amount of energy can be absorbed and cause the spinning proton to flip. =>

$h\nu = \Delta E$

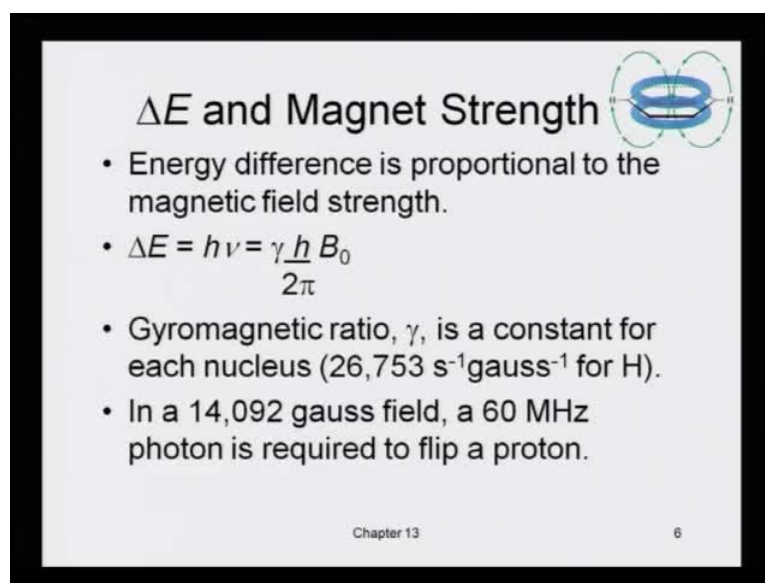
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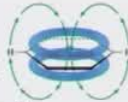
To be able to understand what are these two energy states, let us try to systematically look at every feature of NMR spectroscopy. What actually, is the origin of creating these two different energy states?

The magnetic fields of the spinning nuclei, remember we were talking about a small magnet that have, was generated because the nuclei was spinning and the spin was coming because it has an odd number of electrons, will either align with the external field or will be against the field. So, that is what creates the two energy states.

A photon with the right amount of energy can be absorbed and cause the spinning proton to flip. So, now, if there is a radiofrequency, this brings in a photon of energy and that can either be absorbed by this spinning proton and cause a flip in the, you know, energy level.

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ΔE and Magnet Strength 

- Energy difference is proportional to the magnetic field strength.
- $\Delta E = h\nu = \frac{\gamma \hbar}{2\pi} B_0$
- Gyromagnetic ratio, γ , is a constant for each nucleus (26,753 s⁻¹gauss⁻¹ for H).
- In a 14,092 gauss field, a 60 MHz photon is required to flip a proton.

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Now, this delta E and magnetic strength have a correlation. Energy difference is proportional to the magnetic field strength, so it has to be understood. Only when the radio frequency energy is matching with this kind of magnetic field strength, generated by that spinning nuclei, only then, it will be absorbed. And therefore, delta E is equal to h nu is equal to rho H by two pi B 0.

Now, this is an equation, which is given for the change in energy that is brought about by the interaction of change - from lower energy state to higher energy state. Gyro, gyromagnetic ratio, gamma, is a constant for a nu, for each nucleus and it is expressed as 26753, seconds, per second per gauss per proton. So, you see, that this gyromagnetic ratio is therefore, all these spinning nuclei, that we had seen, the proton 1, the carbon 13, the nitrogen 15 and so on, and they will have a different gamma value for each one of them.

Therefore, in a 14092 gauss field, a 60 megahertz photon is required to flip a proton. So, if the field strength is known and the radio frequency, that is required to excite these nuclei to go from lower energy to higher energy, would be the radio frequency of the range of 60 megahertz.

So, that is the kind of requirement. Low energy, radio frequencies can do the needful.

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Magnetic Shielding

- If all protons absorbed the same amount of energy in a given magnetic field, not much information could be obtained.
- But protons are surrounded by electrons that shield them from the external field.
- Circulating electrons create an induced magnetic field that opposes the external magnetic field. =>

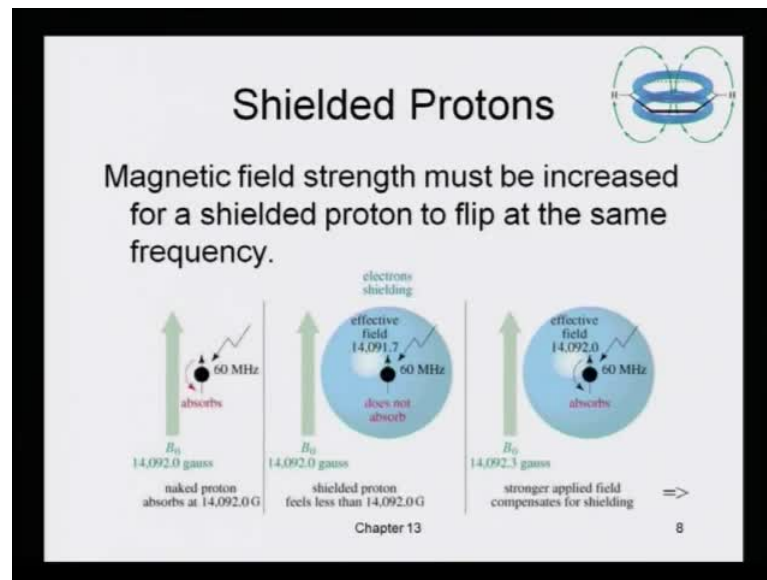
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So, when we are try, and trying to understand, there is something called magnetic shielding. If all protons absorb the same amount of energy in a given magnetic field, not much information could be obtained. Therefore, some of them are shielded and some are deshielded and there is what makes these protons different and because of their chemical environment, that means, the immediate neighbors of each proton are differently placed.

Therefore, the chemical environment becomes different and the magnetic shielding may or may not occur, but protons are surrounded by electrons that shield them from the external field. Circulating electrons create an induced magnetic field that opposes the external magnetic field.

Now, it is not only the role of the proton in the nucleus, but the electrons are actually surrounding them. Now, it is also, they play a, kind of a, shielding effect on the external field, that is being experienced by the spinning nuclei. Now, these circulating electrons create a small induced magnetic field, also because, they are also charged particles and they are also moving, so that opposes this external magnetic field.

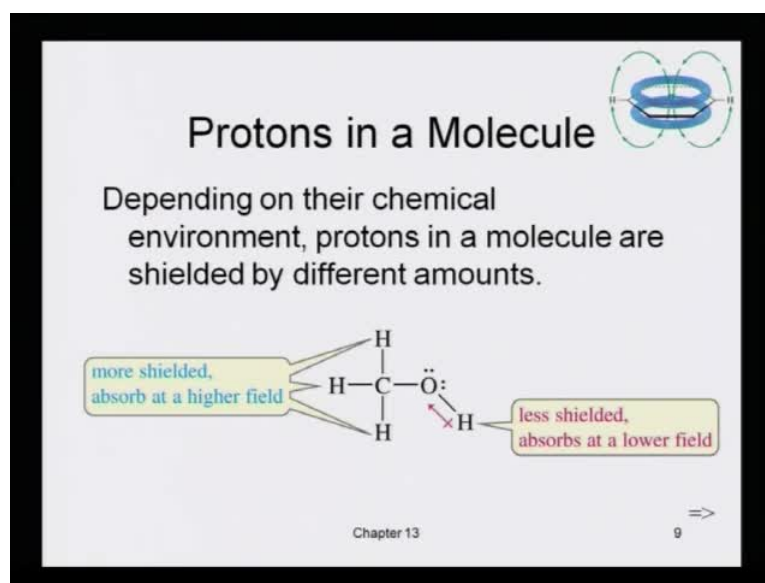
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The shielded protons - magnetic field strength must be increased for a shielded proton to flip at the same frequency. Now, what should happen, that if the nuclei, spinning nuclei is experiencing the effect of the radio frequency under a given larger magnetic group field, which is of the order of 14092 gauss, a naked will absorb at this particular, a naked proton will absorb at 14092 gauss. However, if there are shielded proton, that means, there are, there is a provision of electrons, which can shield, then the same, the proton fields are little less effect of that and the effective field is now 14091, at the same 60 megahertz frequency, radio frequency.

So, you see, stronger field need to be applied to compensate for this shielding because it will not absorb, it is just, you know, getting protected by these spinning electrons. So, therefore, if there is the protons are shielded, one is unshielded versus shielded, unshielded will absorb at the same gauss value but, if there are electrons, which are shielding, it will not absorb. So, a stronger field needs to be applied to compensate for this shielding.

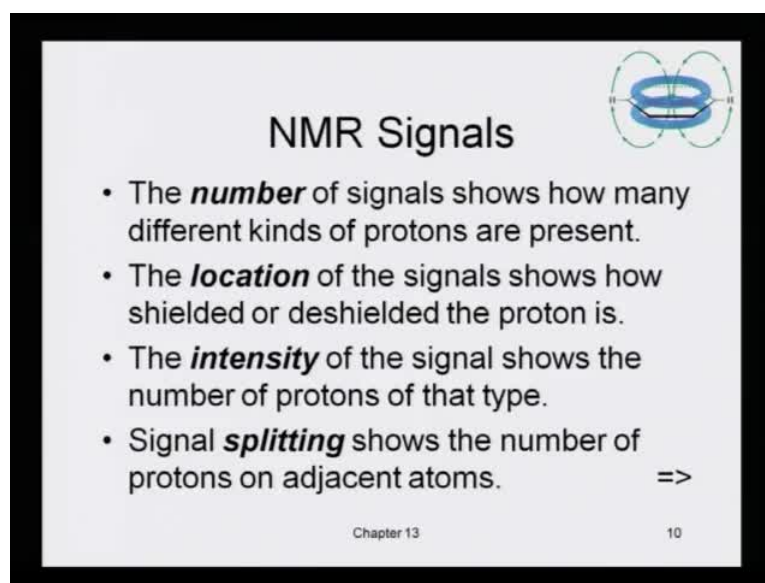
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The protons in a molecule - depending on their chemical environment, the protons in a molecule are shielded by different amounts. So, therefore, more shielded absorb at higher field obviously, because they are experienced. As I told you, that electronic shielding will push them to absorb at a higher frequency of the radio energy and therefore, the more the, such shielding, the higher will be the frequency. Whereas, you look at the simple methyl alcohol molecule, the 3 protons, which are connected to the carbon are more shielded and absorb at higher field, whereas the proton, which is connected to oxygen is less shielded because there is this lone pair and so on and so forth, and it absorbs at a lower field. That makes all the 4, the hydrogens of the methyl alcohol different, otherwise everything will come in the same place and it will be of no consequence for a chemist to understand.

So, if the beauty of NMR is that because of this shielding effect and differently shielding effect of different protons because of their chemical environment. The protons in a molecule are shielded to different amounts and that gives a very informative picture about the structure of a compound.

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A slide titled "NMR Signals" with a diagram of a proton's magnetic field. The diagram shows a central blue circle with two blue loops above and below it, representing the magnetic field. The slide contains a bulleted list of four points: 1. The **number** of signals shows how many different kinds of protons are present. 2. The **location** of the signals shows how shielded or deshielded the proton is. 3. The **intensity** of the signal shows the number of protons of that type. 4. Signal **splitting** shows the number of protons on adjacent atoms. To the right of the fourth point is an arrow pointing right (=>). At the bottom of the slide, it says "Chapter 13" on the left and "10" on the right.

NMR Signals

- The **number** of signals shows how many different kinds of protons are present.
- The **location** of the signals shows how shielded or deshielded the proton is.
- The **intensity** of the signal shows the number of protons of that type.
- Signal **splitting** shows the number of protons on adjacent atoms. =>

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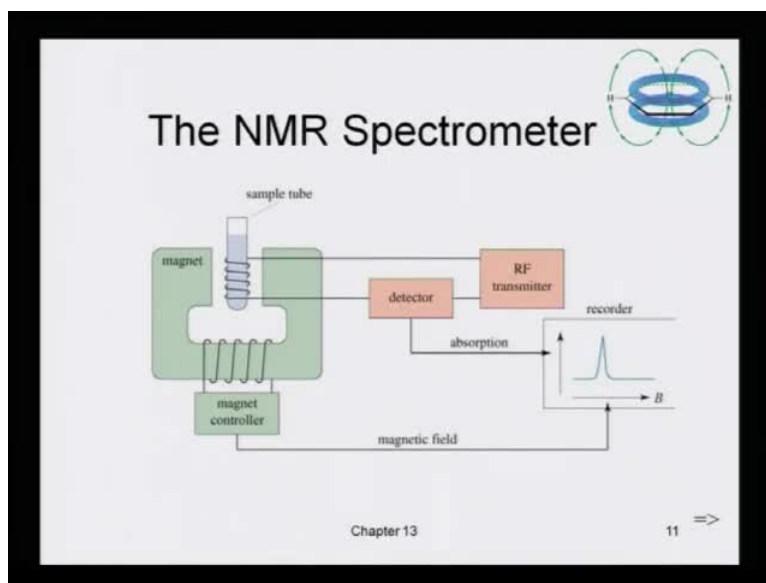
Now, when we try to look at the NMR signal, the number of signals shows how many different protons or different kinds of protons are present.

So, if we try to look at the number of the peaks in, in NMR spectra, that will tell us, how many different, environmentally different protons are present in that molecule? The location of the signal shows how shielded or deshielded the proton is and also in the NMR spectrum, the location of these peaks will give us an idea, whether the protons are shielded or deshielded, as we saw in the case of methyl alcohol.

In the case of methyl alcohol, the methyl protons were shielded, whereas the OH proton was deshielded. The intensity of the signal shows the number of protons of that type. Now, because of this peak getting intensified, if it is 1 proton, the peak will be smaller; if it is 2 protons, it was close to almost the double and if there are 3 protons, the peak will be almost 3 times the peak of 1 proton, so that intensity also shows, or is a signal of the number of protons of that particular type.

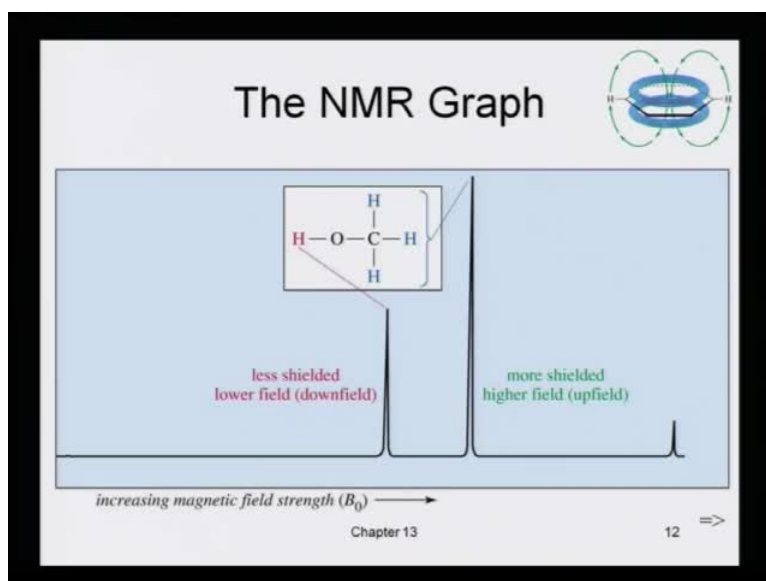
Signal splitting shows the number of protons on adjacent carbon atoms. Now, what happens is that they are locally affected, the adjacent protons are, you know, get affected and they split their peaks. So, the number of splitting, if there is 1 proton on the left-hand side and if there are 2 protons on the right-hand side, the left-hand side will give a triplet and the right hand side will give a doublet; so, that is the kind of splitting, that occurs in an NMR spectra.

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This is how the NMR spectrometer looks like. There is a huge magnet, there is a sample tube and the, there is a RF transmitter, which will create radio frequencies, there is a detector, which will be collecting the information and the detector will then, through the absorption, will go into the recorder, and the magnet actually, is controlled by a huge magnetic field. Therefore, it, this is a very simple pictorial description of an NMR spectrometer.

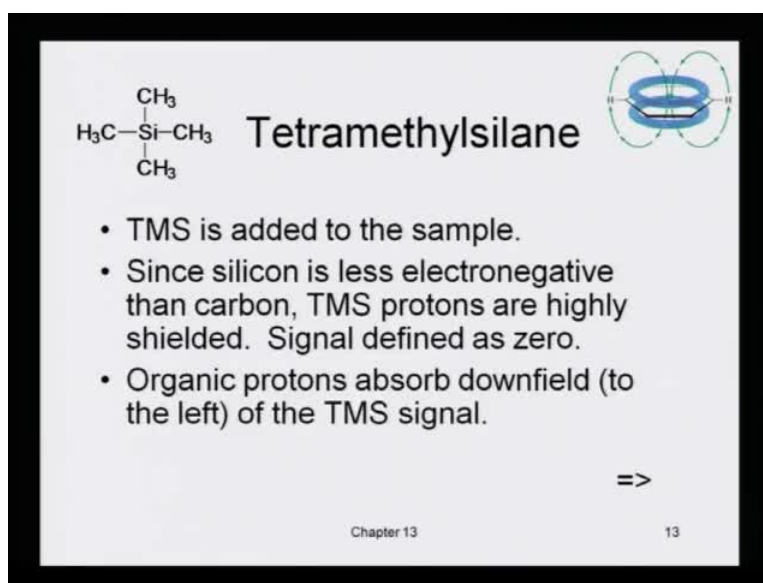
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We do not call it an NMR's photo spectrometer, why? Because there is no light, which is shown, this is of the UV or visible region. Here, the EMR, that is used, that is the electromagnetic radiation, that is used, is of the radio waves and so, it is referred as radio frequency and radio frequencies are always in hertz or megahertz. And therefore, this is not called as a spectrophotometer, but it is the, it is called NMR spectrometer.

Now, when we try to look at the same example of methyl alcohol, you will see, that the less shielded or lower field OH, H will come downfield and the more shielded will come on the upfield. So, what is this upfield, downfield? First, we have to understand, that there is an electromagnetic field strength and in that field strength, whichever comes on the left side is more downshield or deshielded, and the one, which is on the right hand side is, from where the 0 begins, is the more shielded or higher or upfield protons.

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The slide features the chemical structure of Tetramethylsilane (TMS) on the left, consisting of a central silicon atom bonded to four methyl groups. To the right of the structure is the title "Tetramethylsilane" and a diagram of a p-orbital. Below this, a bulleted list explains its role as a reference compound. At the bottom right, there is an arrow pointing right, and at the bottom center, the text "Chapter 13" and the number "13" are displayed.

C[Si](C)(C)C Tetramethylsilane

- TMS is added to the sample.
- Since silicon is less electronegative than carbon, TMS protons are highly shielded. Signal defined as zero.
- Organic protons absorb downfield (to the left) of the TMS signal.

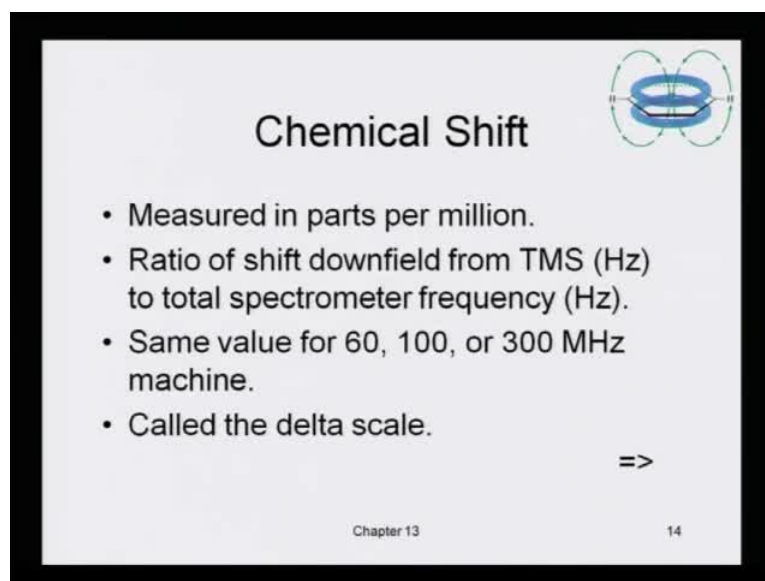
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Now, tetramethylsilane is one compound, which is taken as the 0 end of a scale because we need to scale it up, we need to have a scale against which all the protons will be measured. So, the 0 pointing part is the tetramethylsilane. TMS is added to the sample, why? Because nothing can be lower than TMS and you will see, that in TMS all the protons have the same environment and therefore, it gives only 1 peak. There is no splitting, there is no, you know, different kind of all the methyls are the same and all the protons, all the 12 H are the same. Therefore, it acts as the standard starting point of any NMR spectra.

Since, silicon is less electronegative than carbon, the TMS protons are highly shielded and therefore, they are highly shielded and signal defines as, as 0 organic protons absorb downfield to the left of the TMS signal. So, the added advantage for using TMS as a 0 point is that all other organic compounds will be downshielded or they will be on the left hand side; so, that can be set as a 0 point in NMR spectra.

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Chemical Shift

- Measured in parts per million.
- Ratio of shift downfield from TMS (Hz) to total spectrometer frequency (Hz).
- Same value for 60, 100, or 300 MHz machine.
- Called the delta scale.

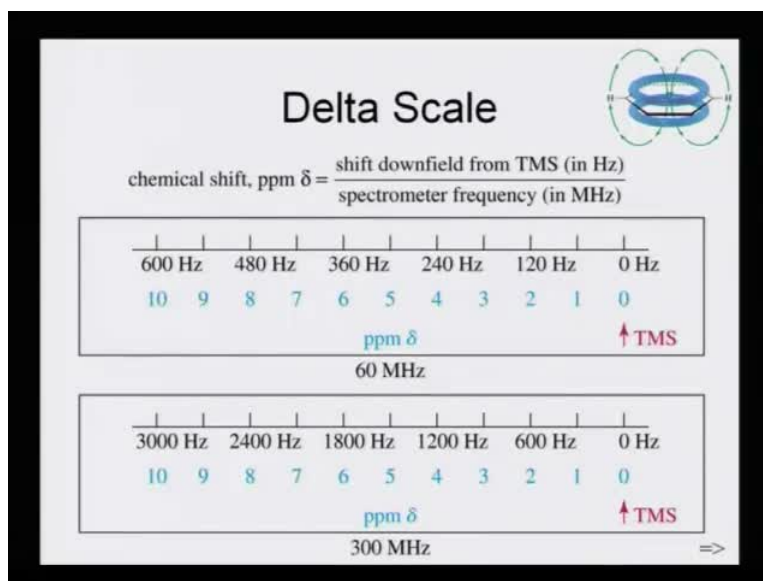
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Now, what are these different chemical shifts and what does this has any relevance in terms of NMR? Chemical shifts, that are actually shown in an NMR are at, are measured in ppm or parts per million; ratio of shift downfield from TMS, that is in hertz, to total spectrometer frequency, which is also in hertz. So, where is it, with respect to TMS, that is called the chemical shift for a particular type of proton, attached to a particular type of carbon or any hetero atom; same value for 60, 100 and 300 megahertz machine.

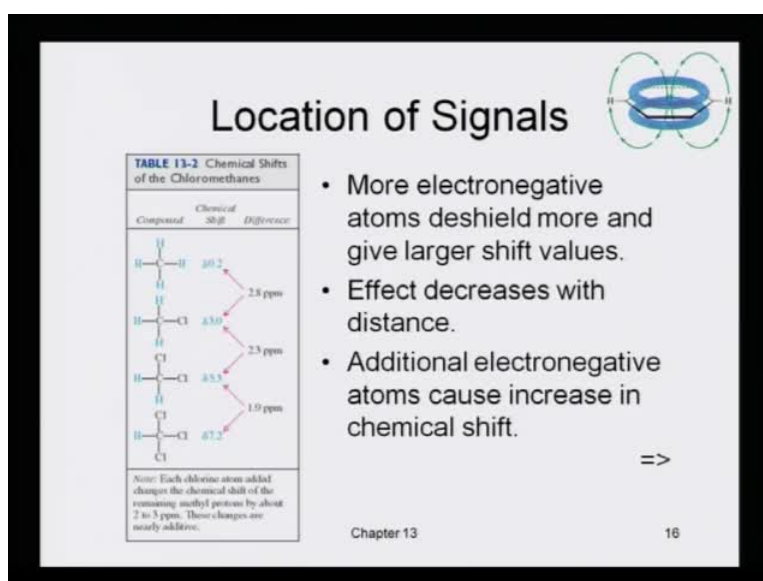
So, the beauty is that the chemical shift value will remain the same even if the radio frequencies are changed from 60 to 100 to 300 megahertz, and this is also called the delta scale, that is, you know, as I said, there has to be a scale setup for NMR and with respect to some 0, these other protons are measured. Whether they are more downfielded or they are more shielded, it is a, or upfielded, will be decided as compared to the TMS value, which is set as 0. So, one need to have a scale. If I say that my height is 5-3 then, there has to be some point from where I am measuring my height. So, the same way, these NMR values are also collected or calculated with respect to the TMS being 0.

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Now, if you try to look at the delta scale, the chemical shift or the ppm or the delta value will be, shift downfield from TMS in hertz upon the spectrometer frequency in megahertz. So, what is the frequency in megahertz and what will be the relative chemical shift? And you will see, that the TMS is always 0 at 0 hertz and then subsequently, as the protons move upward they, or get de-shielded, they are, have different values between, the scale is from 1 to or 0 to 10. For proton NMR, the scale for finding any proton, where 0 is the TMS and it can go up to 10 ppm value or delta value.

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Now, location of signals - more electronegative atoms deshields more and gives larger shift values. So, if you remember certain rules of NMR calculation and also the observable values of differently different protons in different, environmentally different situations, then you will be able to calculate the chemical shifts and identify on the basis of the chemical shifts, which are the protons.

So, looking at the table, you will see that chloromethane have different chemical shifts. There is a possibility, simple methane will show signal at 2.8 ppm, but if there is one chloro group, you will find it at 2.3; if there are 2 chloro groups, then you will find at 1.9 and so on, and so-forth. So, more electronegative groups are attached or atoms, that are attached, create deshielding more and the, it gives larger shift values if it decreases with distance. So, it is only, when it is just neighboring to that particular carbon, which holds the proton, which is under study, the effect will be pronounced. Additional electronegative atoms cause increase in chemical shift; obviously, each one is creating a little bit of shielding or deshielding, so the chemical shift will be altered.

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Typical Values			
Type of Proton	Approximate δ	Type of Proton	Approximate δ
alkane ($-\text{CH}_3$)	0.9		1.7
alkane ($-\text{CH}_2-$)	1.3	Ph-H	7.2
alkane ($-\text{CH}-$)	1.4	Ph- CH_3	2.3
	2.1	R-CHO	9-10
$-\text{C}\equiv\text{C}-\text{H}$	2.5	R-COOH	10-12
R- CH_2 -X (X = halogen, O)	3-4	R-OH	variable, about 2-5
	5-6	Ar-OH	variable, about 4-7
		R-NH ₂	variable, about 1.5-4

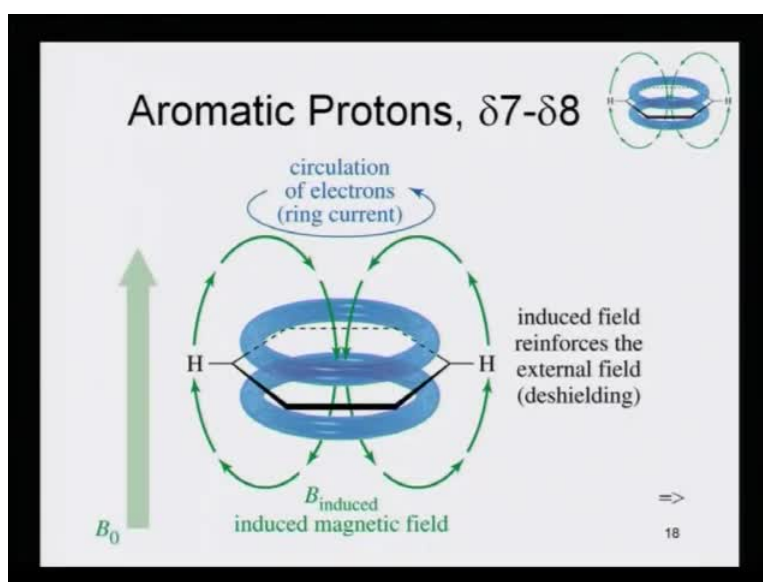
Note: These values are approximate, as all chemical shifts are affected by neighboring substituents. The numbers given here assume that alkyl groups are the only other substituents present. A more complete table of chemical shifts appears in Appendix I.

So, if you try to look at different protons and also try to look at the approximate delta value, a simple alkane proton will appear at 0.9; alkane, which is you know, substituted on both the sides or may be the CH₂ of the alkyl group, then it will appear at 1.3; if the alkane is substituted furthermore, it will appear at 1.4 and so on.

Similarly, if you have a carbonyl attached to an alkyl and that alkyl is under study, it will appear at a delta value of 2.1, and if it is an acetylenic proton, it will appear at 2.5; if it is a, you know, if a halogen is attached to the CH 2, then it will appear between 3 to 4 and if it is a double bonded proton, it will appear between 5 to 6 delta value. So, almost like the functional groups of IR, like the chromophore groups of UV, these have definite delta values. So, if there is a peak appearing and these, one can immediately identify, that such a group must be a part of the molecule.

Similarly, if there is a **methyl** group attached to an olefinic bond, there is a change to be, that methyl will appear at 1.7; simple **methyl** does not appear at 1.7, it appears at 0.9. So, you see, that shift has occurred because of the olefinic bond that is in continuation, so that is causing the de-shielding to occur. A fennel proton, that means, an aromatic hydrogen will appear at 7.2 basic value, but if the same phenyl is, hydrogen is substituted by a **methyl**, then this **methyl** will appear at 2.3. So, you see, a simple **methyl** was appearing at 0.9, with the double bonds in conjugation made it to switch over a, get deshielded to 1.7 and furthermore, if it is attached to a benzene ring, the value goes up to 2.3. So, that is the kind of variation that the delta value has because of the immediate environment in which the proton is placed.

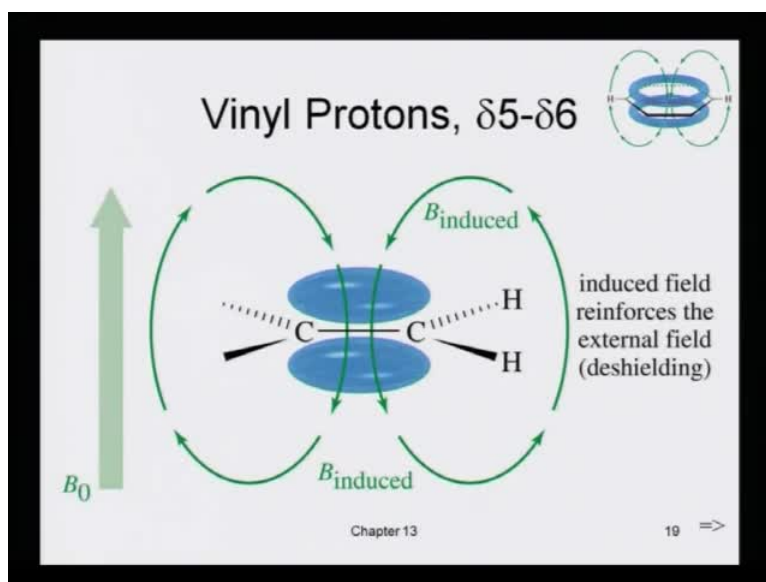
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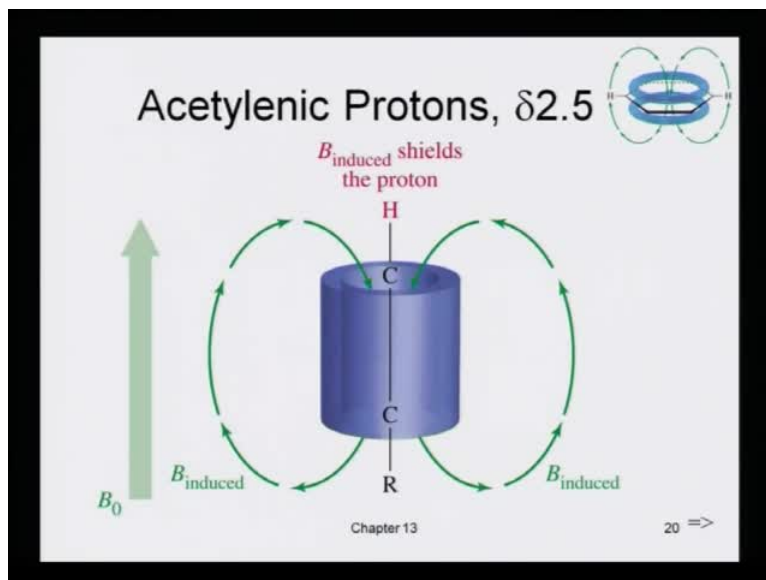
So, if we try to look at the aromatic protons, why do they show such drastic shifts, is because there is a circulation of electrons of the ring current and then there is an induced

magnetic field. The induced magnetic field reinforces the external field thereby, causing a deshielding effect and that is why, it goes further beyond from the TMS and the value from 0.9 goes to point, 2.3. So, that is the kind of de-shielding that these circulating electrons or the pi electrons create for the nuclei of that aromatic ring.

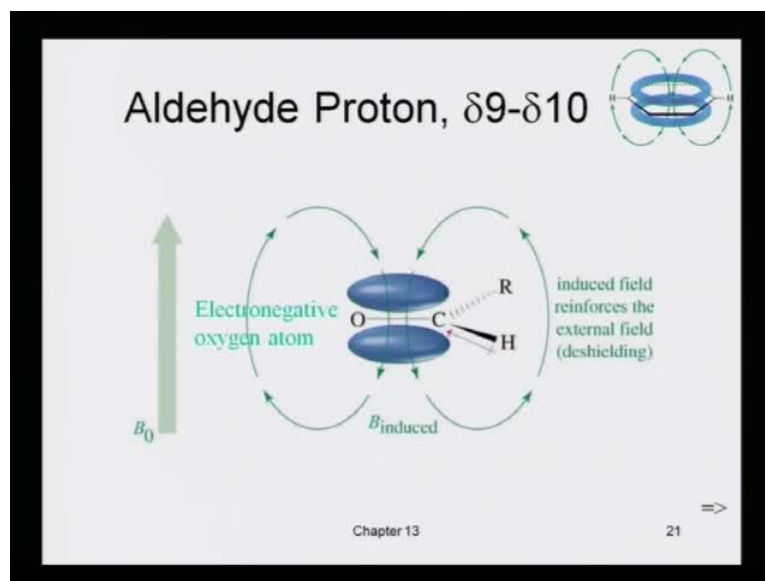
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Similarly, vinyl protons also show delta value between 5 and 6. Now, again, they create an induced field, which is, which reinforces the external field and therefore, they are deshielded to such an extent, that it goes up to 5 to 6 ppm, or delta value acetylenic protons also have a similar kind of induced deshielding and therefore, it is shifted between delta value 2.5 or so on. Similarly, aldehyde protons get furthermore deshielded because of the electronegative oxygen atom, which reinforces furthermore, the external field de-shielding and therefore, the value goes up to 9 to 10.

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O-H and N-H Signals

- Chemical shift depends on concentration.
- Hydrogen bonding in concentrated solutions deshield the protons, so signal is around $\delta 3.5$ for N-H and $\delta 4.5$ for O-H.
- Proton exchanges between the molecules broaden the peak.

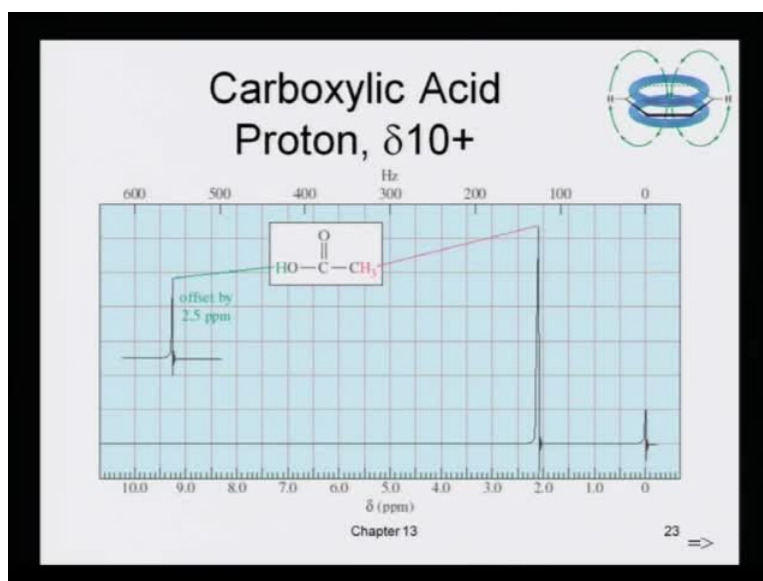
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So, that is how the environment is changing, the deshielding is affected. Proton exchanges between the molecules broaden the peak. So, these O-H and N-H signals are very, very typical cases, where the chemical shift depends on the concentration. Hydrogen bonding in concentrated solution deshields the protons, so signals are seen around delta value 3.5 for N-H and 4.5 for O-H. So, you see, furthermore, because of the electronegativity of oxygen being higher than nitrogen, the delta values are 3.5 and 4.5 respectively for amines and hydroxyl groups.

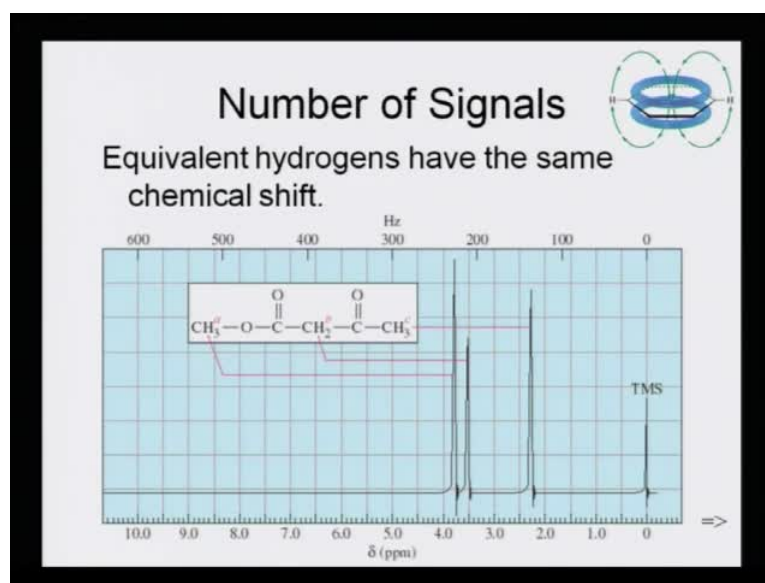
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So, if we try to look at the carboxylic acid, the proton comes at delta, almost close to 10 or sometimes even above 10. And that, if we take a simple example of acetic acid, it has only 2 types of proton, one belonging to the carboxylic group and the other one belonging to the methanol group.

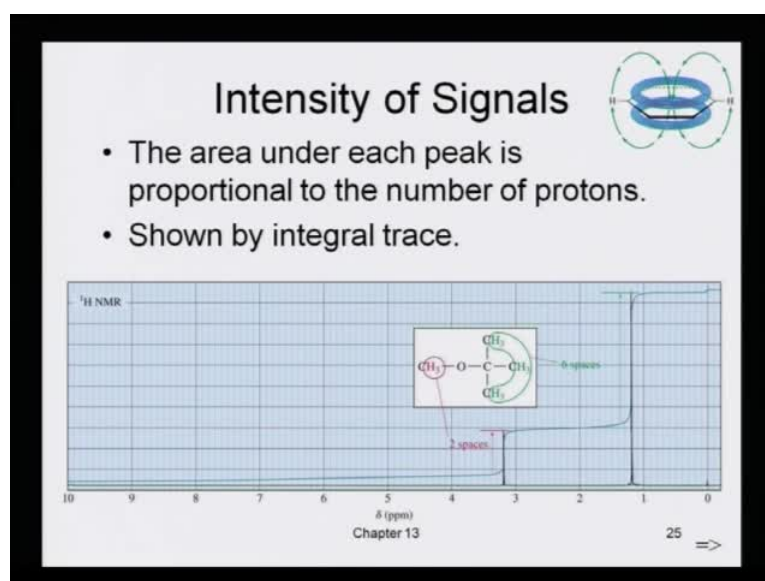
Now, the one, which is the **methyl** group, is so much deshielded by the effect of the carbonyl next to it, that instead of coming at 0.9, it is now appearing at 2.1 and the carboxylic proton appears at between 9 to 10 delta value.

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Number of signals - equivalent hydrogens has the same chemical shift. This is, if you try to look at this particular example of $\text{CH}_3\text{COCH}_2\text{COOCH}_3$, acetoacetic ester, you will see that TMS of course, is set at 0, then there is this **methyl** C proton, then there is this CH_2 and then there is this CH_3 , which is next to the carboxylic, rather carboxylate and therefore, all the 3 protons, different types of protons, that true **methyls** are different and the CH_2 **methylene** is different, can be seen very correctly in this particular NMR spectra and very clearly, they are remarked as different signals altogether.

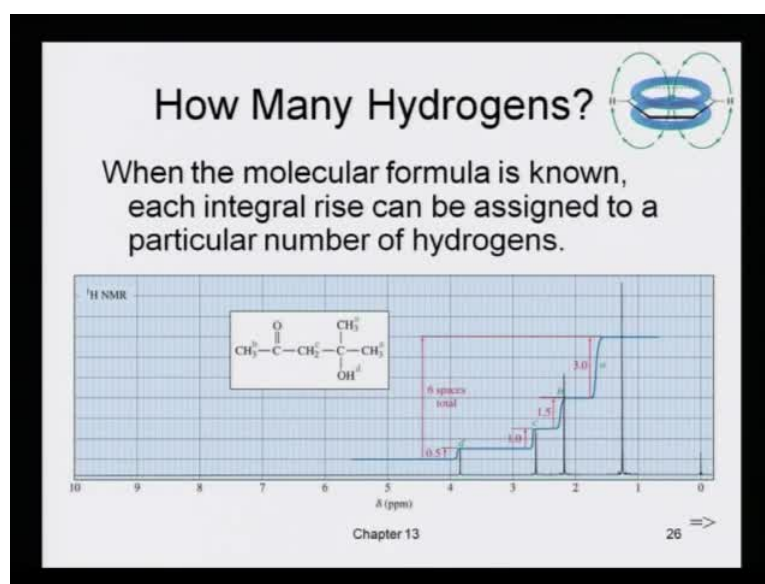
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The area under each peak is proportional to the number of protons, so that is also varying good, that one can calculate the number of protons very effectively by taking the area under which the peak appears.

Shown by integral trace - there is a possibility to integrate the spectra and therefore, one can find out, what is, how many spaces in a graph it is covering and in, if you take this example, you will see that 6 protons or rather 9 protons are of one type and 3 protons are of one type, but the ratio is 1 is to 3. And therefore, if this is occupying 2 spaces, we are, the one must occupy 6 spaces to be able to justify, that it is 3 times more than the previous or the more deshielded proton.

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How many hydrogens? When the molecular formula is known, each integral rise can be assigned to a particular number of hydrogen. So, because we understand, that every proton has its proportionality, therefore it is possible to calculate the total number of hydrogen in a molecule. Because of this integral rise, if one is showing 0.5, the other one is showing 1, the 3rd one is showing 1.5 and then, last one is showing 3. That means, they are in that proportion appearing, so the total number of hydrogens of protons can also be calculated for a molecular formulae very easily.

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Spin-Spin Splitting

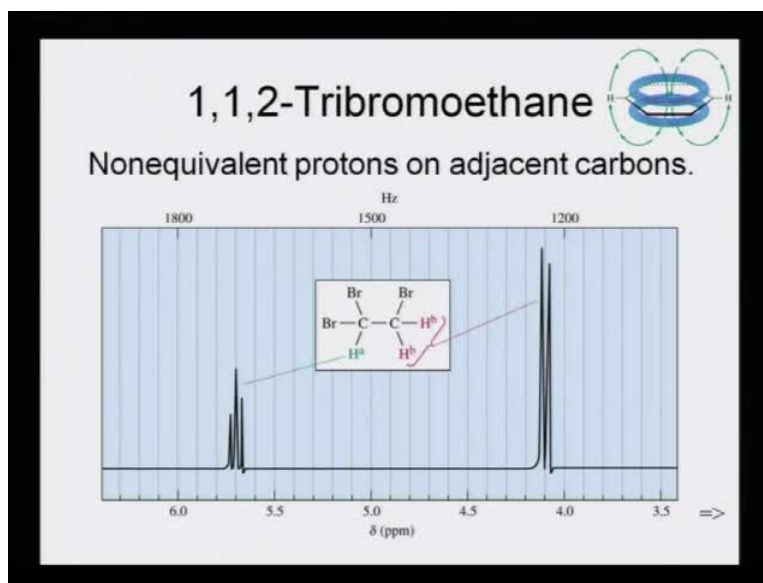
- Nonequivalent protons on adjacent carbons have magnetic fields that may align with or oppose the external field.
- This magnetic coupling causes the proton to absorb slightly downfield when the external field is reinforced and slightly upfield when the external field is opposed.
- All possibilities exist, so signal is split. =>

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Spin-Spin splitting - non-equivalent protons on adjacent carbons have magnetic field that may align with or oppose the external field. So, furthermore, what happens is that when they are nonequivalent protons on the adjacent to carbons, then they can create more spin splitting and therefore, have a magnetic field, that may align or oppose them external field. So, again, that creates the unsymmetry, let us say, non-equivalence of the protons on the adjacent carbons, can cause splitting.

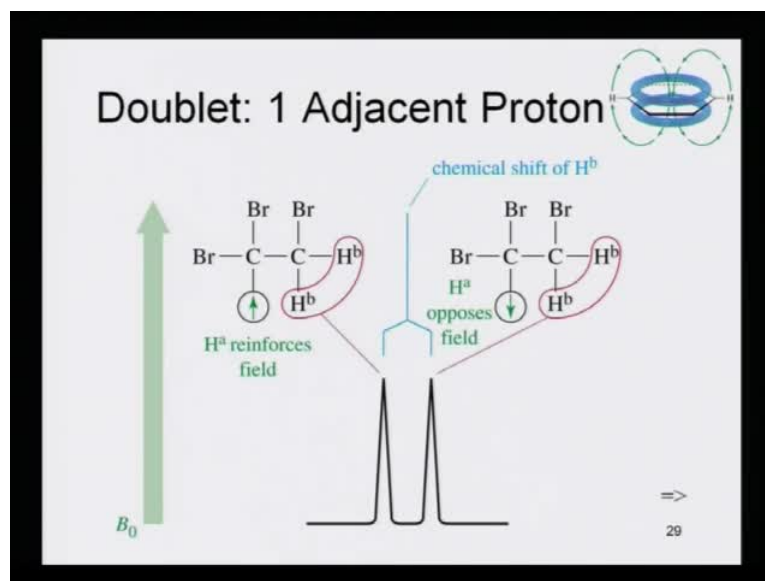
Now, what is this Spin-Spin splitting? This magnetic coupling causes the proton to absorb slightly downfield, when the external field is reinforced and slightly upfield, when the external field is opposed. So, quite rightly, this particular magnetic coupling causes the proton to absorb slightly on the downfield when the external field is reinforcing, what we saw in the earlier case and it will slightly move downfield, if the external field is opposing. All possibilities exist, so signals are split.

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Now, you see, this is a very nice NMR spectra of 1,1,2-Tribromoethane, so that there are only 2 types of protons, one is the H a and the other one is H b, but the H a is experiencing the effect of the, splitting effect of the H b, which are 2 in number, so it will appear as a triplet, whereas the H a is in the, Hb is looking at only H a. Therefore, they will appear as a doublet. The example that I gave a while ago, that non-equivalent protons on adjacent carbon, can create this kind of splitting; they look at the neighbor and accordingly the splitting takes place. If the neighbor is 2, the splitting will be 2; if the neighbor is 1, but they themselves are 2, then it will be a triplet. So, that is how, the splitting takes place.

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The doublet, 1 adjacent proton - because of this H^a being reinforced by the H^bs, there is a splitting, that occurs and there is a chemical shift, that occurs because of the H^b. So, it is because of these adjacent protons, which are causing splitting.

So, in, in simple words if I have to explain to you, they look at the neighboring carbon and the protons, that are sitting in the neighboring carbon and causes the splitting to occur because of the, this field being reinforced or opposed and therefore, one finds this kind of situation.

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The N + 1 Rule

If a signal is split by N equivalent protons, it is split into $N + 1$ peaks.

Number of Equivalent Protons Causing Splitting	Number of Peaks (multiplicity)	Area Ratios (Pascal's triangle)
0	1 (singlet)	1
1	2 (doublet)	1 1
2	3 (triplet)	1 2 1
3	4 (quartet)	1 3 3 1
4	5 (quintet)	1 4 6 4 1
5	6 (sextet)	1 5 10 10 5 1
6	7 (septet)	1 6 15 20 15 6 1


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So, there is a thumb rule, which is called N plus 1 rule for the splitting pattern. If a signal is split by N equivalent protons, it is split into N plus 1 peak, if 1 is seeing 2, then it will cause N plus 1, so it will cause a triplet; if 2 are seeing 1, it will cause a doublet; so N plus 1 is the thumb rule. So, if there are number of equivalent protons causing splitting, if it is 0, then only 1, singlet; if there is 1 proton, then it will cause doublet because N plus 1; if it is a 3 equivalent protons, then it will cause quartet, so on and so forth.

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Range of Magnetic Coupling



- Equivalent protons do not split each other.
- Protons bonded to the same carbon will split each other only if they are not equivalent.
- Protons on adjacent carbons normally will couple.
- Protons separated by four or more bonds will not couple.

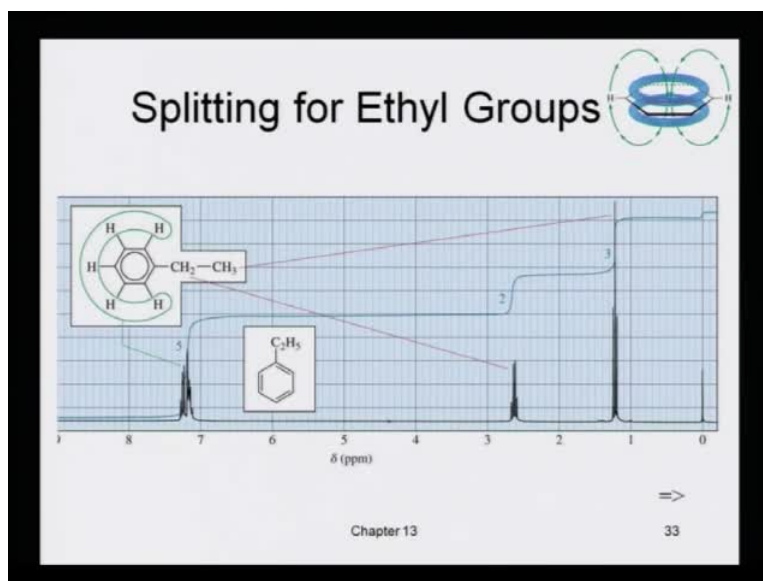
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Range of magnetic coupling - equivalent protons do not split each other. Protons bonded to the same carbon will split each other only if are not equivalent. Protons on adjacent carbon normally will couple and protons separated by 4 or more bonds will not couple.

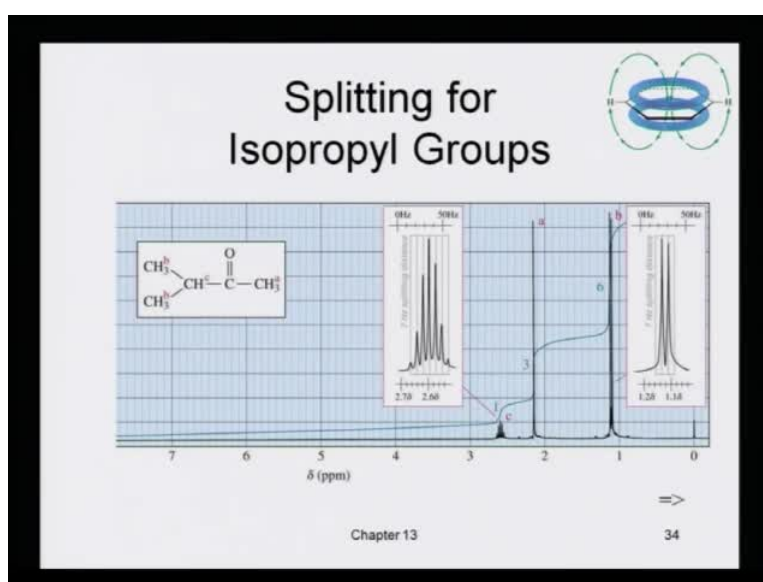
So, there are some very basic rules of molecular, magnetic coupling. It is not that, all protons will get affected by all protons. If they are further away, they will not affect. So, proton separated by 4 or more bonds will not couple will not cause any kind of splitting. Protons on adjacent carbons normally will couple, that is the only rule that has to be remembered. Protons bonded to the same carbon will split each other only if they are not equivalent. Now, if the **methyl** of the 3 protons of the same carbon, will not affect each other, it is the adjacent carbon proton that is affected. So, equivalent protons do not split each other. So, these are certain basic rules that need to be remembered, while looking at the splitting pattern of the NMR spectra of protons.

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Splitting of ethyl group – now, if we try to look at this ethyl benzene, you will see that the CH₂ causes the splitting pattern of the 5 protons that are present on the benzene ring. The **methyl** causes splitting of the ethylene protons, which is CH₂ and vice-versa. So, there is a complex kind of triplet, quartet and a multiplet, which is depicted nicely by these 3 different varieties of protons residing on different areas of the molecule.

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Splitting for isopropyl group - if there is a compound like this, there is an isopropyl means, there are 2 **methyls** attached to CH, **methyne** and that now makes it different.

These 2 CH 3s are different from the CH 3, which is next to the carbonyl and therefore, one should expect 3 different types of protons in 3 different areas and therefore, one would find 1 intense peak near 1 ppm, another intense peak near 2 ppm and a very small multiplet between 2 and 3. Now, there is multiplet, which is between 2 and 3, is the actual CH methyne protons whereas, the one, which is between 2 and 3 is because of the isopropyl **methylyls**. And if you try to look at the integration, you will find, that the integrations show, that the values are 1 is to 3 is to 6 and therefore, it is a typical case of the isopropyl group splitting very beautifully and showing a multiplet.

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Coupling Constants

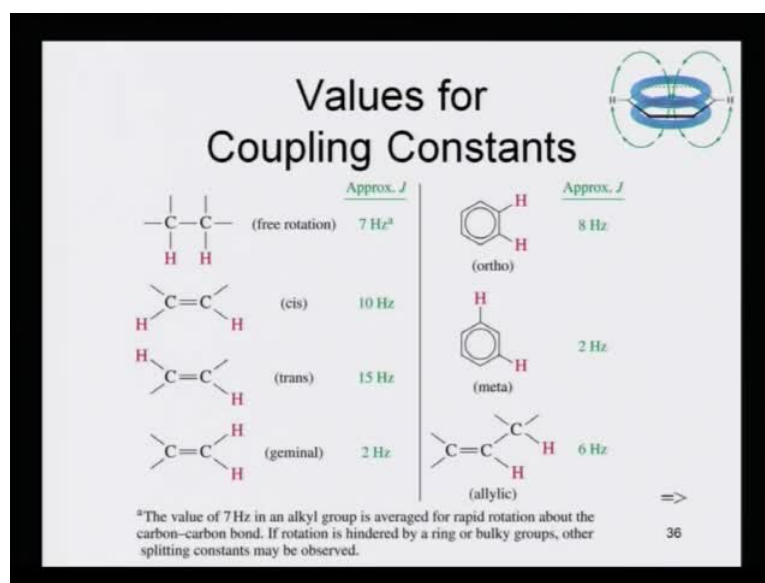
- Distance between the peaks of multiplet
- Measured in Hz
- Not dependent on strength of the external field
- Multiplets with the same coupling constants may come from adjacent groups of protons that split each other.

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Coupling Constants - distance between the peak of multiplet is also a very important criteria when we try to look at an NMR spectrum, measured in hertz and not dependent on the strength of the external field. Multiplets with the same coupling constant may come from adjacent groups of proton that split each other. So, coupling constant is again a very important feature of an NMR, as I said a while ago, and it is the distance between the peaks of multiplet, that means, within a multiplet, what is the, and the distance between each peak and it is measured in hertz and it is not dependent on what is the external field, because the splitting will occur and the coupling constant will remain, as the one name suggests, constant. Multiplets with the same coupling constant may come from adjacent groups of protons that split each other.

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Some of the values of coupling constants are given here. If we try to look at a simple alkane, the 2 protons on the adjacent carbon, because of the free rotations have approximately, a coupling constant of 7 hertz. But the 2 protons of a cis **alkane** will have a coupling constant, because here it is restricted, so 10 hertz, whereas the coupling constants of 2 protons, which are trans to each other will have a j value of 15 hertz. And protons of geminal type, which are under same side of the double bond, will have a very low coupling constant, that is, 2 hertz.

The value of 7 hertz in alkane is average for rapid rotation about the carbon-carbon bond. If rotation is hindered by the ring or bulky groups or other splitting, constants may also be observed. So, you can see, that the 2 hydrogens in a benzene ring, which are ortho to each other, have a coupling constant of 8 hertz; the 2 hydrogens, which are meta to each other, have a coupling, I mean, do not couple at all, so they have a coupling constant very low as 2 hertz. And another allylic situation, where there is an alkene, which is restricting, will have coupling constant, **of the acetate**, of the ethene ring and the **methyl** proton as 6 hertz.

So, these are some of the coupling constant, that is, where to find, what would be the distance between the 2 splitting peaks is what is known as the coupling constant and it is, it gives a lot of information about the arrangement of protons in a molecule.