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**Course Title
Advanced Characterization Techniques**

Lecture-14

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Today we are going to discuss about a new spectroscopic technique that is called infrared spectroscopy.

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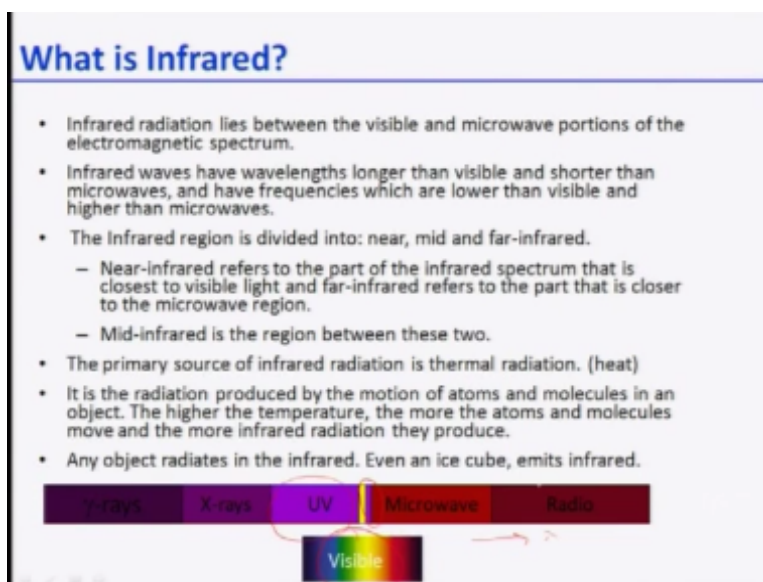


Infrared spectroscopy is part of these the advanced chemical spectroscopic techniques which are used to determine different kinds of chemical information, starting from the electronic transition to the vibration spectroscopy to even the nuclear transitions. So this normally used in the machines as a Fourier transform infrared spectroscopy or something known as FTIR. So if TIR is

the major Fourier transform technique which is normally used in the experiments and whenever you go to any such labs they will talk about FTIR.

The full form FTIR is Fourier transform infrared spectroscopy. basically is an infrared spectroscopy but the information which are obtained from the machine are basically plotted in this Fourier space instead of the real space and furiously pace is nothing but the wave number space. Now this is this spectroscopic technique that our infrared filters techniques it deals with the infrared region of the electromagnetic spectrum and I will first give you an idea what is infrared radiation is.

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Now as you know infrared radiation is lies between visible and the microwave portions of the electromagnetic spectrum. The very first class I just showed you the detail in for it is the lintel spectrum of the rectum and radiation we are studying form x-rays or gamma rays to radio waves are shown and whether you be invisible comes in the middle of the of the spectrum. So infrared which crumbs which between the visible and the microwave that is this one here, so you can see this is the part visible microwave.

We have already discussed about the EV and the visible spectroscopic in the last class, so here the wavelength comes basically falls between these two the spectrums infrareds are normally have higher wavelengths than the visible as clear blends increases in this direction. So let λ

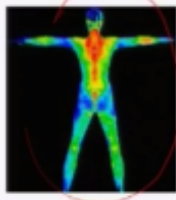
increase in this direction and the frequency of will decreases as you go from EV to microwave radio.

Infrared instance indigo and basically divided into three parts, one is a meeting for it that is exactly the infrared radiation region and then you have a near-infrared and the falling for it. Near-infrared means the part of the infrared spectrum that is closest to the visible light and far-infrared means the part which is closer to the microwave religions and mid-infrared obviously is between these two are the middle of that.

Primary source of this info radiation is thermal which I will discuss in the next slide that is basically heat, now this is radiation is produced by the motion of atoms and molecules in an object higher the temperature more the atoms and molecules move and more the infrared radiation is. So any objects radiates it radiation in the infrared regions even an ice cube actually inter a d its infrared radiations.

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What is Infrared? (Cont.)



Humans, at normal body temperature, radiate most strongly in the infrared, at a wavelength of about 10 microns (A micron is the term commonly used in astronomy for a micrometer or one millionth of a meter). In the image to the left, the red areas are the warmest, followed by yellow, green and blue (coolest).

The image to the right shows a cat in the infrared. The yellow-white areas are the warmest and the purple areas are the coldest. This image gives us a different view of a familiar animal as well as information that we could not get from a visible light picture. Notice the cold nose and the heat from the cat's eyes, mouth and ears.



So to give an idea humans at normal body temperatures radiate most strongly in the infrared region that is why, there are cameras developed to get images in infrared spectrum and these cameras are very popular for the night photography and they know this most of the human beings at normal body temperature radiate strongly enough around a table and about 10 microns. And in the image which is shown here in the left part of this figure is the basically the you know here the areas which are red and yellow are these highest temperatures regions as you can see that.

On the other hand this right side picture source and night picture night image of a cat using infrared radiations, yellow white areas are the warmest, so you know why it is I is actually at a very high radiation coming from the face and the paw pads are the coldest. So this kind of imaging techniques are widely used for the photography of in the night are even some time in case of the other things.

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Infrared radiation

$\lambda = 2.5 \text{ to } 17 \mu\text{m}$
 $\bar{\nu} = 4000 \text{ to } 600 \text{ cm}^{-1}$

These frequencies match the frequencies of covalent bond stretching and bending vibrations. Infrared spectroscopy can be used to find out about **covalent bonds** in molecules.

IR is used to tell:

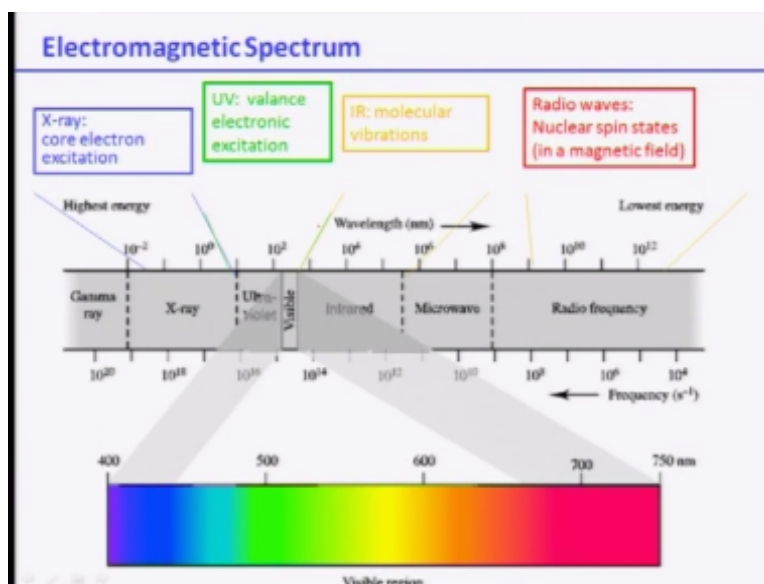
1. what type of bonds are present
2. some structural information

So I am going to show you the actual values of the infrared radiation surveillance and the wave numbers, so ever lamps are false in the region of 2.5 to 17 micron that means they are quite large even it compared to the visible ones are actually, I know 400 to 800 nanometers. So if you multiply this one with nanometers that means if you multiply with 10^{-3} so it is basically 25 to 1700,

So sorry two 2150 nanometers is much higher than the visible and the corresponding wave numbers are basically four thousand to six hundred centimeter inverse, these frequencies match frequencies of the covalent bonds basically in the material or in the molecules ever stating in the pipe earlier the bending vibrations. So you have a covalent bond like carbon carbonyl carbon hydrogen or carbon oxygen covalent bonds.

There the these frequencies actually match very well with the stretching and bending vibration of those points, so therefore one can it will mean the kind of bonds presents inside a covalent bonding material, this is why it is very widely used for covalent bond molecules. So infrared radiations are in fact spectroscopy is normally used to tell you what type of bonds are present in the material and also some type are a structural information which will show you as you go alone.

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So they give an idea why does it lie as I said you this lies between visible and the microwave the frequencies actually falls in the region of 10^{12} to 10^{14} s^{-1} and the wavelengths are about 1 mm to 100 μm and so therefore they talk about the molecular vibrations and this have indicated can be studied we already discussed about you visible which can be used for valence electronic transitions and so I am basically complementary technique as compared to the UV visible.

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IR Spectroscopy

The IR Spectroscopic Process

1. The quantum mechanical energy levels observed in IR spectroscopy are those of *molecular vibration*
2. We perceive this vibration as heat
3. When we say a *covalent bond* between two atoms is of a certain length, we are citing an average because the bond behaves as if it were a vibrating spring connecting the two atoms
4. For a simple diatomic molecule, this model is easy to visualize:



Vibration of a Diatomic Molecule
Approximates an Oscillating Spring

Now to give better spot perspectives of this infrared spectroscopic process actually deals with quantum mechanical energy levels, which are similar to the molecular vibrations. So I do not have time rather to go into the quantum mechanical treatment of the molecular structure I hope you have already studied in your different courses, like fixed metals or maybe some other quantum mechanical courses. So I understand that these techniques are basically this quantum contentment of molecules gives you the idea of the different quantum mechanics energies.

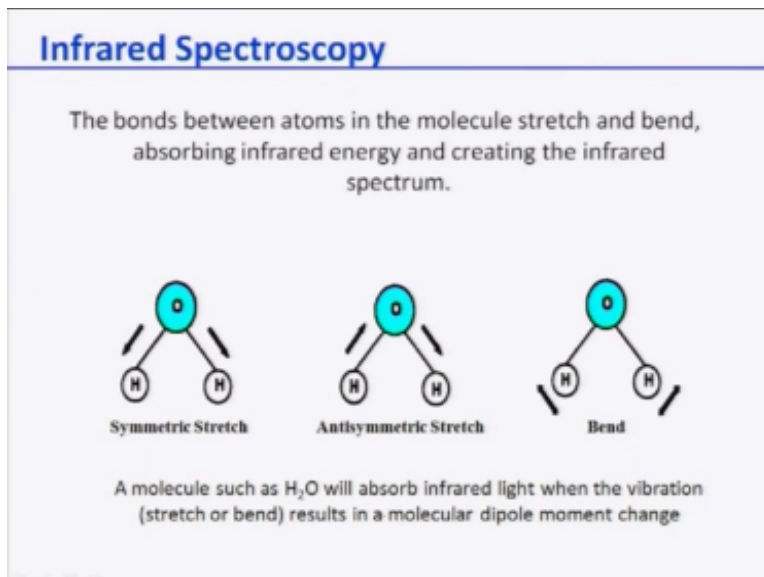
And we know that there are different quantum numbers starting from principal quantum numbers to my naughty corner lambdas, to as even the quadrant us to spin quantum numbers they indicate the different energy levels. So and as in this case actually quantum mechanics energy levels which are used or rather in spectroscopy are basically similar to the molecular vibrations. Now we perceive this vibration in terms of heats actually, so that means some kind of heat that is what I showed you some pictures few minutes back.

Where we can image the animals or even human using infrared spectra camera, when we say a covalent bond between two atoms is a certain length we are citing an average because the bond behaves as there is a vibrating not remitting atom. Let us see the picture here a big item the small atom the bond between these two actually can be thought of it is not basically like a spring. Spring a vibrating spring which is connecting them, so that means molecules are vibrating a certain manner I say the atoms of habitation module certain manner.

But simple molecule is a diatomic molecule you can be easily model this kind of situations using this picture, so if that is the case that means I know we know that for any spring there is a vibration the speak when C which is very unique to the spring and if we know the vibration speaker frequency, we can know the energy and if once you know that a G we can clearly say that if you see the infrared radiations we can analyze this spring to the higher energy level.

And when it comes back to ground level it limit the radiation which is absorbed and by that by measuring that we can determine type of bond presence into the another mark in the material. So now you know as I said bonds between the atoms in a molecule can stretch can bend when it absorbs infrared energy and that saw actually.

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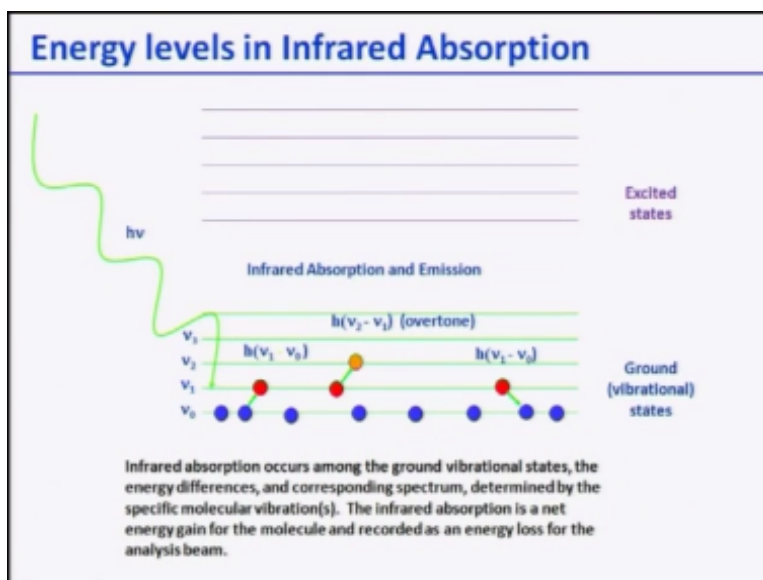
The inference the whole plot between the infrared between the absorption or the transmissions versus wavelength cannot prepare here, so to give you some idea this is called systematic stretch I will show you some even a nice reduce systemic stretch means you have suppose oxygen to hide an atom this like water molecule. So there will be systematic stretch in these two bonds oxygen atom bonds.

You can have an asymmetric stretch to the Appalachian infrared like this to a different direction Pharaoh's are you going to bend that means you can basically the hardened bottoms actually can move little weight or other fibroid little bit this way and then that can create append. So molecules such as water actually can absorb infrared light when Prohibition results in a

molecular dipole moment change this is very important as far as the info spectroscopic concerned.

Because that is how we can actually tell lies this technique to determine what kind of particular you know vibration is present even in the water molecule itself.

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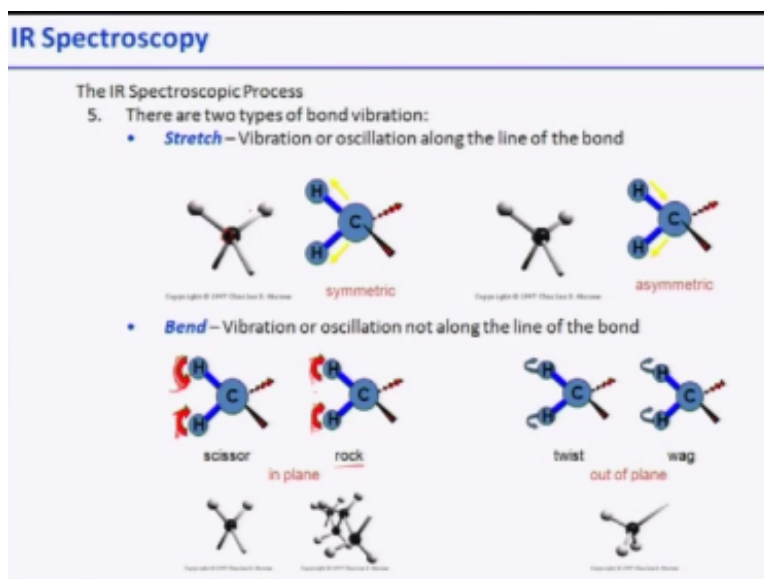
To give you a better idea let us consider but there are any kind of you know atomic energy levels and in the atom these are the ground state its evaluation of ground states you can clearly see these are the atoms blue color atoms are staying there and these are the excited states. Now we apply certain wavelengths of infrared energy what is going to do? These atoms which are presents here they will absorb this okay and when they absorb they get to the excited States suppose they vibrate from μ_0 to μ_1 .

Even if you apply more energies from μ_1 to μ_2 okay, so in as the time goes on these atoms which are excited to the μ_1 frequencies can come back to the down state and leaving behind infrared emissions, if you pump in more energy these items can go into this energy states high on the excited states and even then they can come back. So when they will come back there will be huge change of energy and that a times you will come and say radiations and that is what is been written here.

Absorption app basically occurs among the given personal states in energy difference and the corresponding spectrum determined by the specific molecular vibrations that is what is important. The influence absorption is need energy given for the molecule and recorded as energy loss for their analysis beam.

So molecule absorbs energy gain energy because it is absorbing from the infrared input radiation and as a result of which this energy loss analysis beam that means the beam which is coming out from the material a private interaction will be it i will be energy loss that can be determined easily. Yes as I said I will show some very nice videos, so as you can clearly see the different dynamics and bends switch.

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This all taken from Charles and Atkins which is this book classic book by these two authors as you can see the stretch is basically symmetric where atoms can symmetrically move, this is I to let me put you this is suppose carbon atoms and there are four hydrogen atoms and I am just putting

to harden atoms, they are on here and they are moving symmetrically. So there is a symmetric stretch this is one kind of vibrations and this perishing will lead to certain kind of energy and vibration frequency also be defined that is $\mu_0 \mu_1 \mu_3$.

And if you suppose if these two bonds are moving opposite to each other at a particular time like when this one is moving out this is moving in, so because of that there will be a symmetric vibrations that is also possible they are different states of energies okay. So when I am a infrared radiation falls on it that can it can modify this kind of stretch vibration along the line of the bond next one it can modify the bend.

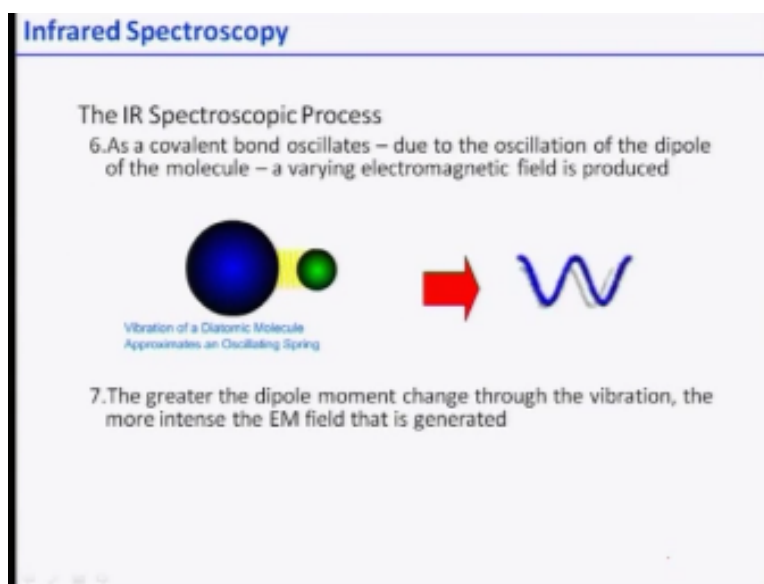
Now you can have a different kind of Bends the one which is shown is this basically in plain bend, it can be either scissor type of rocking type scissor time means suppose in this case both hardened atoms are moving in the same directions, so therefore there is a seizure type is you know scissor both the scissor whenever we use a scissor to cut certain things both this you know but scissor pieces they come and meet at the with the same directions.

Other one is called rocking, rocking means they are actually moving in the same opposite direction sorry in scissor case these two atoms are moving in the opposite directions not in the same direction that is why they can come scissor actually they come in opposite directions. In a rocking case these two atoms are moving in the opposite directions one is this sorry this top is more atoms are moving the same directions because they move in the same direction there is a rocking aspects and this happens in the when atoms are moving the same plane if the atoms are moving in out of the plane.

So the first situations in this case like Caesar which correspond to twist okay that will be twisting the bonds second one who is called wag that is both the atoms are moving the same directions so that will lead to wag so you can clearly see that these are all soon here and Caesar is this like this and rocking is like this and this is a thing twist so these situations will lead to different kinds of energy state.

So the molecule that is what I am trying to impress you up on so that you can you can actually use this kind of energy levels to detect the kind of vibration, vibration is special in the molecule that is why it is called vibration spectroscopy I spectroscopy is always known as a vibration spectroscopy to be greater you give you an better perspectives aspect.

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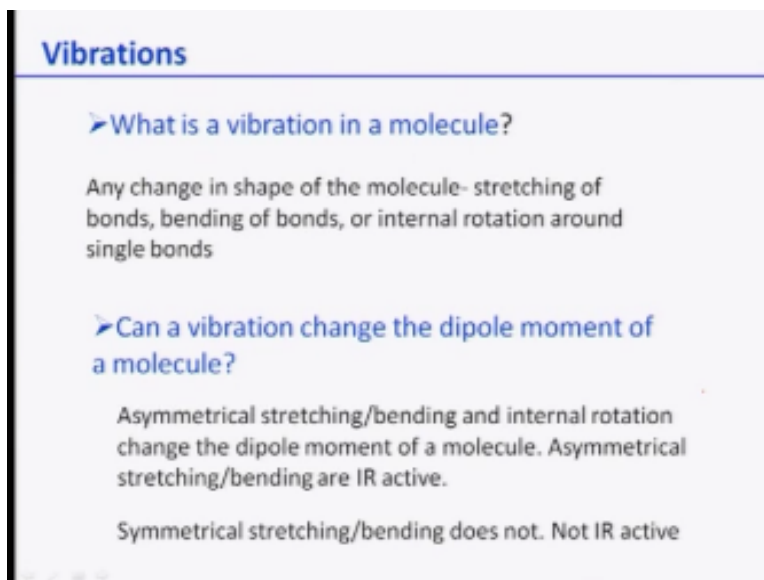


To ski passes actually you know as a covalent bond oscillates due to oscillation of the dipole of the molecule okay sup this two are actually dipole a varying electromagnetic field is produced and because of that you can see there is a propagation of the radiation and get a dipole moment change the vibration and the more intense will be the electromagnetic field an added an electromagnetic field means there is prohibitions.

So that is what is normally is basically classically can be used now when a wave of infrared light encounters any accelerating electromagnetic field shattered by this dipole up same frequency the two cup waves can couple and then when the two waves couple that means the IR edition which is coming and the electromagnetic field which is generated by this accelerating dipoles they can couple and when they couple actually this couple wave can vibrate with the double.

The amplitude of the initial wave that is what is shown here so you can see they are elect this is the input and this is the because of the electromagnetic field and when the couple you have electromagnetic wave which is very, very you know double the amplitude.

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Vibrations

- What is a vibration in a molecule?
Any change in shape of the molecule- stretching of bonds, bending of bonds, or internal rotation around single bonds
- Can a vibration change the dipole moment of a molecule?
Asymmetrical stretching/bending and internal rotation change the dipole moment of a molecule. Asymmetrical stretching/bending are IR active.
Symmetrical stretching/bending does not. Not IR active

So this all can be direct used so this is again same things which has told you I am just going to rush you through this so this all vibrations vibration means stretching a bond spending of bonds internal notations which I have shown you already and then vibration can see the dipole moment I also saw Saudi with a symmetrical stretching or bending or maintain rotations the swag it can change the dipole moment of molecule symmetrical stretching or bending bass not normally so they are not active to the IR radiation.

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Vibrations

What wavelength of electromagnetic radiation is involved in causing vibrations in molecules?

Infrared (IR) electromagnetic radiation causes vibrations in molecules (wavelengths of 2500-15,000 nm or 2.5 – 15 μm)

For a vibration at 4111 cm^{-1} (the stretch in H_2), how many vibrations occur in a second?

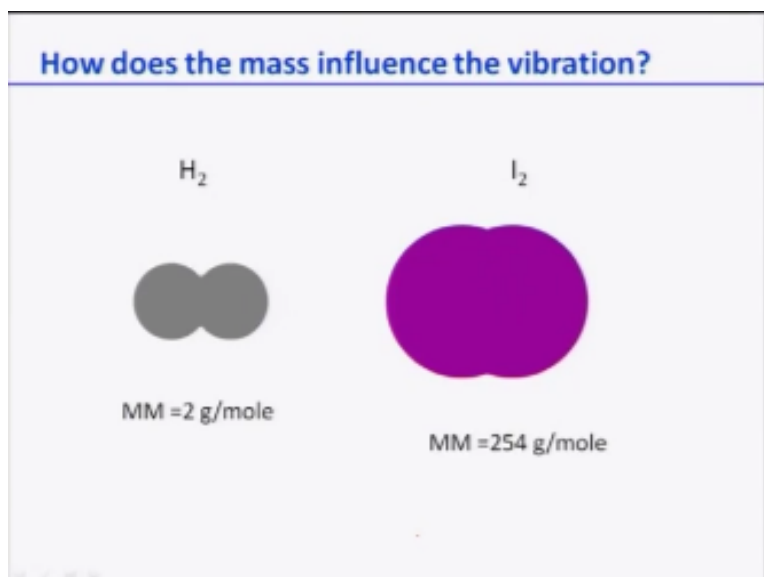
120×10^{12} vibrations/sec or a vibration every 8×10^{-15} seconds!

Now you know normally why the what is the kind of vibration level so wavelengths I have already told you wavelengths should be of the order of 2500 2 17 15 to 17 a thousand nanometers okay now vibrations if you have vibration of suppose 4101 11centimeters inverse that is in stage case of h2 molecule.

So can you imagine how many vibrations can help is done in past second it is very, very large it can be of the order of 120×10^{12} vibrations per second that means one valuation / 10^{-15} seconds which is sometimes is very difficult to detect that so you have Auto second laser spectroscopy we can where you can use infrared laser.

And using auto second laser Pacific spectroscopy you can determine each of this variation auto second means ever minus 18 second so the spectroscopy which is done at the timescale can be used to detect this kind of vibrations which is now a routine nowadays many labs in this even our country has this kind of spectroscopes.

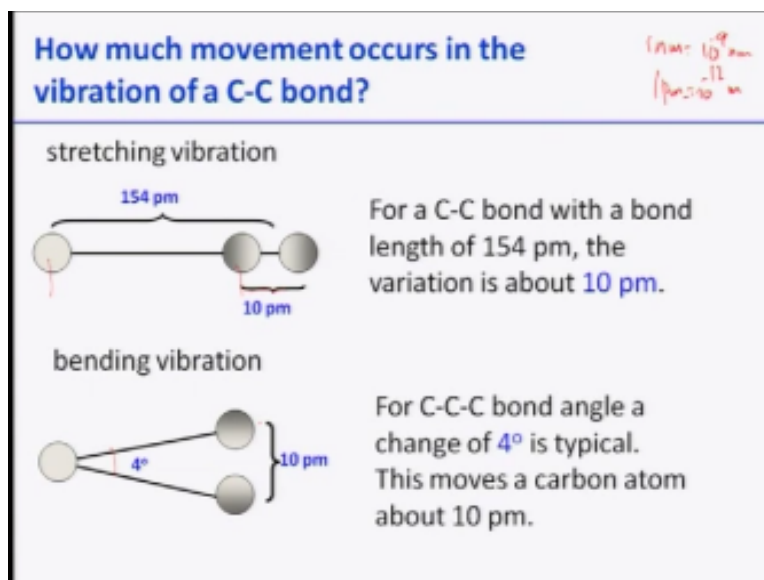
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So this is a very large spectroscopy and now I have not told you about one thing this fine this vibration stretching everything is very fundamental to the spectroscopy this actually gets influenced by the mass, mass of the molecule to give you some idea suppose this is a hydrogen molecule this is the iodine molecule has a molecular weight is 2 grams per mole.

And for the iodine is 254 grams per mole huge, huge molecule mass compared to the hydrogen now if you look at it the idea is carry the mass while the wave number sorry for the vibrations to happen this is also very important you must try to remember this.

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So how much is the movement that happens of course a vibration of this C-C point now let us look at even these knitting ET subtitles of that if I consider this suppose this is the one atom carbon atom this is our atom okay so if they vibrate approximately what is the main oh lengths to which it can vibrate that distance extra distance is approximately 10 Pico meters and at the bond length about 150 for pedometers that is what happens.

So for a C-C bond of the bond and the 150-pound 54 micrometers one picometer is it over minus 12 meter because we know one nanometer is 10^{-9} meter so that means if the bond distances are length is our 154rekha meters so that means is equal to almost like Oh point one five nanometers the vibration is even much, much lower it is about 10 picometers so that is a distance Kayla I am talking about it stands for the stitching for the bending what is the bending angle well.

If we consider the carbon-carbon bonds penny angle is maximum 4 degrees so this much of Bend happens when the Moloch 11 the carbon-carbon bonds actually reprobates events the forwarding is that means distance about four of the 10 picometers for SI bonds angle is obtained is our four degrees is very difficult and these moves the carbon atom about 10 p committees.

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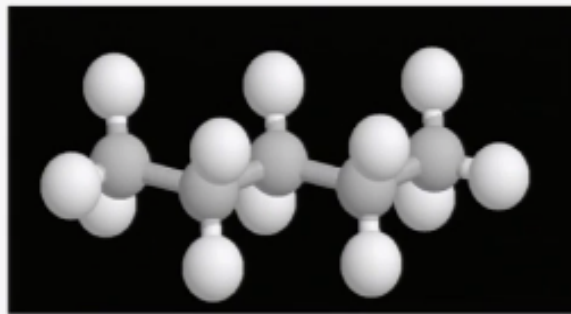
A little physics of electromagnetic radiation

- Energy (E) $E = h\nu = hc/\lambda = hc\nu'$
 - where h is Planck's constant, c is the speed of light, ν is frequency or the number of vibrations per second and λ is the wavelength
- Wavenumber (ν') $\nu' = 1/\lambda$
 - given in cm^{-1}
- Period (P) $P = 1/\nu$
 - the time between a vibration

So I will not discuss about these aspects because I have already discussed with you about energy and the wavenumber and other things.

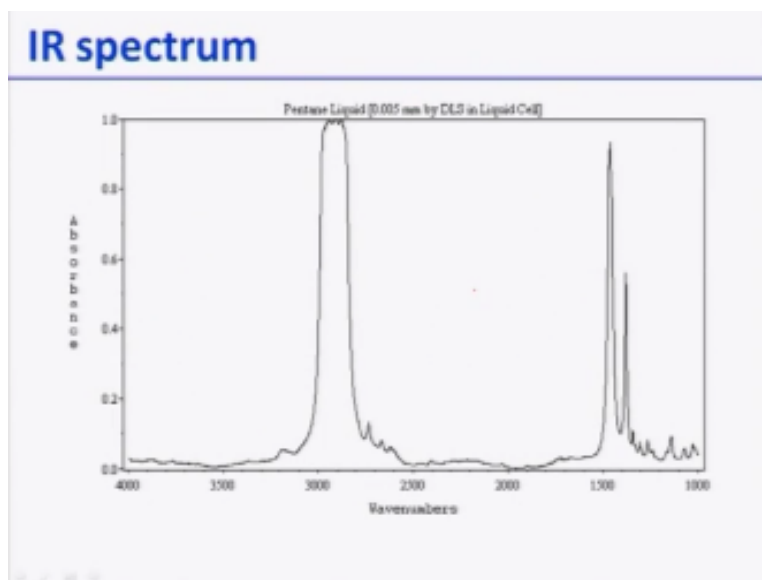
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What type of vibrations would occur in pentane?



So let us look at even a big molecule like Pentane okay pentane is C_5H_{12} okay so there are five carbon atom 1 2 3 4 5 and then there are one two three four five six seven eight nine ten eleven twelve hundred atoms so if this is the case then what kind of type of vibration would occur in this big molecules for small molecules is easy okay examine this.

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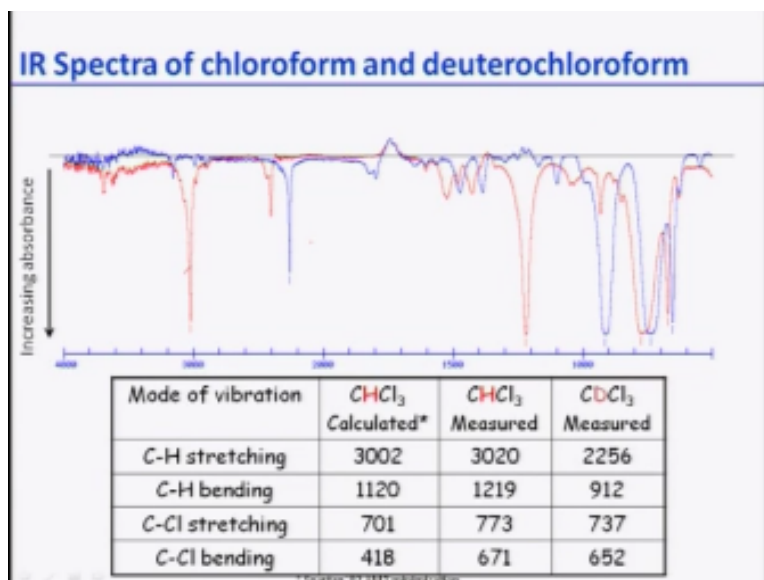


That can be done using by taking the I a spectrum this is panel liquid and this measured using if TR you can see this is the absorbance absorptions this is the wave number and this is absorption a plotted here so you can see the picas coming in this picture their background and pics coming in the pictures are tentative numbers the small Peaks there are big Peaks okay.

And by looking at this peak positions one can actually easily ram in that kind of you know questions which have already asked that vibrations what kind of vibrations will take place in this molecule so increasing the absorption of higher radiation that means as you go Oh 0.221 absorptions what happens see this is Paris a Khaleesi stretching and this is for serious stretching and this is Percy is bending two separate things because as you have seen here.

So I let like to go back we have carbon so this is hydrogen this is carbon this is suppose carbon this is carbon hydrogen bond and this is carbon, carbon bonds that is the overall picture in a pentane molecule so this is saturated what is cos a serrated polymer okay or alkanet rather and so therefore if I look at it this is stretching this particular what is a coming c is stretching and this is CH pending and that is what we can clearly see.

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In case of pentane now if you look at chloroform and even dr. chloroform, chloroform is very common molecule this is taken from this source as you can see the chloroform is basically shown in the red and daughter clap ham Estonian blue so there are certain frequencies for the vibrations we can see so what you can do is that waveform you know chloroform is nothing.

But chcl_3 that means there are 1 h & 3scar chlorine bonds see sequel CCL CCLCH 2 types of bonds so CA stretching for chloroform comes around 2000 to this is this is almost like this okay this part and CH bending CH bending comes either 120 so that is this and CCL comes about seven hundred thousand nine hundred, hundred 700, 700 and CCL bending comes for an 18 summer here comes it is a fair it can be detected.

Similarly for and these are the major values these are normal addicted we can we observe we can see these things and for CDCL_3 that is go to the chloroform okay these are the values and this we detect all of them so therefore one can actually clearly say from these measurements what kind of a now vibration states of the bonds presents in the in this case the speaks shift is because of h_2d and that is because of mass increase.

So you can see that h_2d because of that speak has shifted this week has shifted this the suddenly discussed the mass increase means more mass means the pics will come at a higher up numbers so our web numbers not have some more results.

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Some results

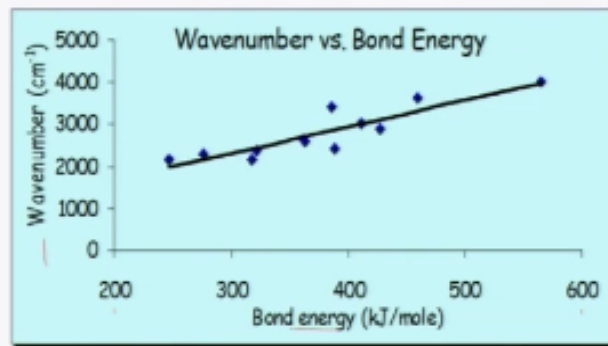
- Calculated values using computational software give **lower** wave numbers
- Increasing mass of substituted atoms shifts wave numbers to lower values
- Stretching energies > bending energies > internal rotation energies (occur at higher wavelengths)

So you know calculated values normally in this cases are had to be compared with computational values which are normally done using computational tools so calculated values as I showed you here in this case calculated values at this and these are the measured values so there is little bit of variations but still one can get this value results very close to it from the Coptic measure value with the calculate value using better compression of tools.

Nowadays which is done and second thing is increasing the mass will ship the way numbers to lower values that is what I told you and third ones teaching energy always had in the bending energies that we also learnt and many hands will be always other than the rotational internal energies which can occur actually higher planes which is normally observe.

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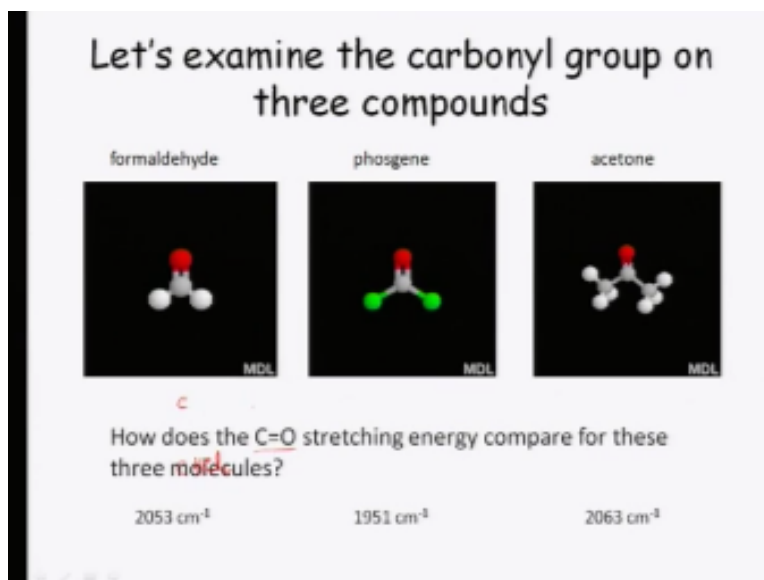
Does the stretching energy have any relationship to the strength of the bond?



So therefore thus the stretching relationship next question have to ask is the teaching lessons energy have any relationship with strength of the bond actually it is true in the two if you look at number versus bond energies so one angle is starting from 200 to about 600 kilo joule per mole where numbers zero to five thousand as you can see that as the bond energy increases wave number also increases.

So that mean searching energy is related to the strain of the bond as the bond increases once increases the staging energy also increases that is what this is called plot at Lisa listing the sort is the case so we can plot it and we can get a very reasonable numbers of the confidence using a square well.

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Now we can actually go on looking at different kinds of molecules and do that most of them will be today's lecture will be up carbon type this is formaldehyde it you know formaldehyde CH_2O to pray and this is phosgene of this acetone we know that and so we will examine this carbonyl groups here so how does this $\text{C}=\text{O}$ bonds cos double bonds here sorry this one everywhere is ever $\text{C}=\text{O}$ double bond.

Okay everywhere you have a $\text{C}=\text{O}$ double bond that is in the all the cases so how does the $\text{C}=\text{O}$ stretching energy compared with this molecules here easily its wave number is 2053 because the force then is it basically 1951 in case of acetone it is even higher 2063 Sandoval universe so that means depending on the structure from CH_2O aldehyde force gene or acetone the $\text{C}=\text{O}$ bond stretching energy will change thus understand.

Because the environment is changing the type of atoms present in the near the $\text{C}=\text{O}$ bonds as it changes the $\text{C}=\text{O}$ stretching energy also changes so carbonyl group normally has energies between 1700 to 3000 centimeters.

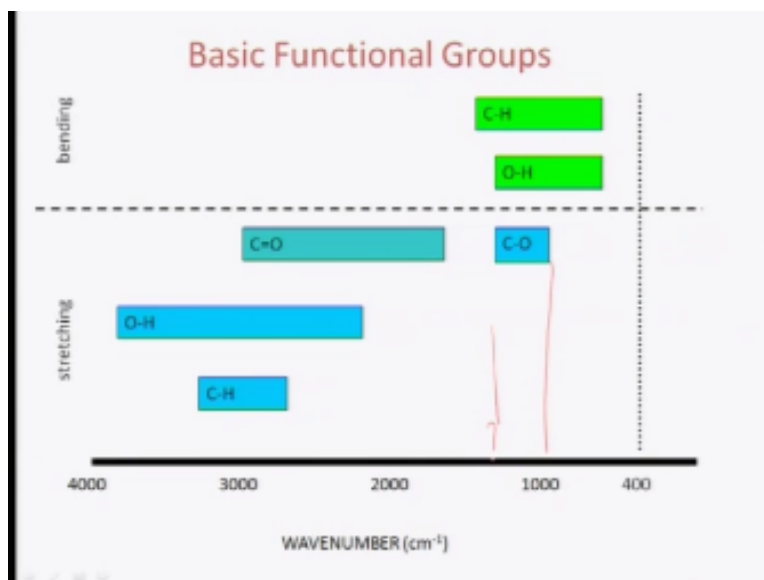
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Functional group analysis in organic compounds

- Unlike atomic spectroscopy where sharp energy transitions occur due to well quantized electron transitions, molecular spectroscopy tends to show **bands**.
- Molecular vibrations are influenced by the surrounding groups!

Now one can actually analyze different functional groups in organic compounds like Atomics unlike Atomic spectroscopy where the spectrum is not as well defined as electron transitions molecular spectroscopy tends to show bands we have seen that different kinds of stretching bands molecular vibrations are normally influenced by these surrounding groups we have seen one example in the last slides.

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So let me just tell you in a brief what we can understand from this kind of spectroscopy this is stretching and bending energies and these are the wave numbers so for a CH stretching energy wave number comes around 2900 but bending will come around one thousand two couple of hundreds of H that is in well groups the stretching energy can span from 4,000 to about 2000 where are bending energy can span from about 1000 to 2000 1500 to about 500 and then sue co is co means double bond o that is the norm formaldehyde acetone all this molecule has this kind of bonds there.

This is the stretching energy can span from three Hudson to about 2500 and your what is called the other type of the sea you actually single bond can happen actually this chasing can happen even at lower wave number that is 1000 1200 to about 1000 and in this case is there are other things like CC double bonds this alkenes and it can happen in the range of about very close range about 1500 and then we can also, also have CC single bonds and this can happen even at much lower row of numbers that is close to 1000.

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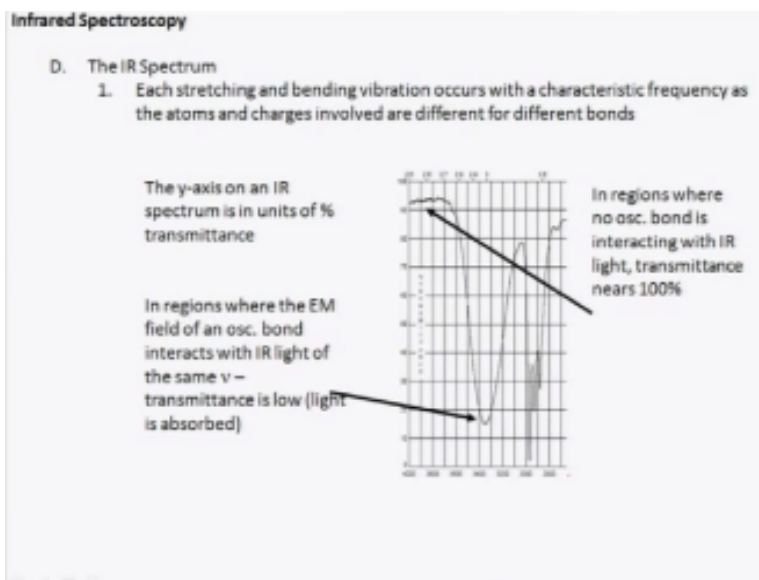
Use of IR spectra

- Identification of functional groups on a molecule - this is a very important tool in organic chemistry
- Spectral matching can be done by computer software and library spectra
- Since absorbance follows Beer's Law, can do quantitative analysis

So using the IR spectroscopy actually one can determine these this kind of bonds let us see that what else we can do so therefore we can actually identify different functional groups in a molecule that is very important player organic chemistry because you need to know what kind of function group is present in the molecule which is produced by the chemical reactions and then only you can basically formula structure of the molecule spectral matching can be done by computer software.

As I told you even library spectroscopic data also available seen this, this absorbs and follows Beer's law you can actually do quantity Malice's also I already discussed you would be a slow in first lecture even in case of visible invisible spectroscopy also how to apply that and one can actually use this law and then do quantitative analysis also to do that.

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Let us see that okay and this is basically another kind of representation and you know I teach I have told all these things already to you but let me reallor it each staging and bending vibrations actually occurs has very specific characteristic frequencies which we have already told you and as you can see that this actually where the prefab electromagnetic field law acceleration sinter actual the aisle lights.

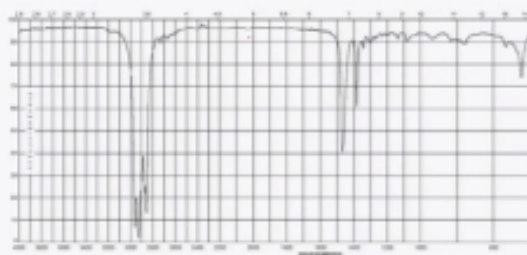
So transmission very low this is basically transmitting spot entire not the absorptions passes wave number and region where these acceleration bonds inductor is light the termination is almost like one hundred percent this is the ones so that means there is no acceleration so bonds so there is no transmission.

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IR Spectroscopy

D. The IR Spectrum

2. The x-axis of the IR spectrum is in units of wavenumbers, ν , which is the number of waves per centimeter in units of cm^{-1} . [Remember $E = h\nu$ or $E = hc/\lambda$]



This is again another kind of plots for transmissions vs. wave numbers and we can see different bands stretching and the bending bands we can determine that for different molecules.

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IR Spectroscopy

D. The IR Spectrum

- This unit is used rather than wavelength (microns) because wavenumbers are directly proportional to the energy of transition being observed $\bar{\nu}$
chemists like this, physicists hate it
High frequencies and high wavenumbers equate higher energy
is quicker to understand than
Short wavelengths equate higher energy
- This unit is used rather than frequency as the numbers are more "real" than the exponential units of frequency
- IR spectra are observed for what is called the mid-infrared: $400\text{--}4000\text{ cm}^{-1}$
- The peaks are Gaussian distributions of the average energy of a transition

And to give you some more ideas about it normally respect terms okay uses you need to have the no I blends because so even numbers are tightly purposing to the energies as you have told because is new is the energy and this can be written as $h\nu$ by λ so $\bar{\nu}$ new bar is the energy say where new bar is basically the wave number so wave number is directly proportional to the energy not the wavelength of llama is inversely proportional to the energy that is why we plot it higher frequency have numbers are equate the higher energy so equate the high energy that is why we use the UF numbers and web numbers are extensively use I do not want to tell detail about that.

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Infrared Spectroscopy

E. The IR Spectrum – The detection of different bonds

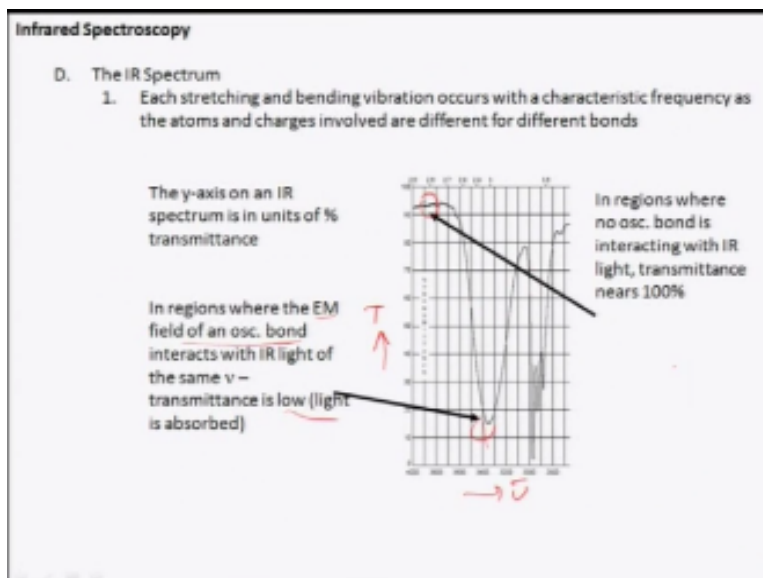
9. It is important to make note of peak intensities to show the effect of these factors:

- **Strong (s)** – peak is tall, transmittance is low (0-35 %)
- **Medium (m)** – peak is mid-height (75-35%)
- **Weak (w)** – peak is short, transmittance is high (90-75%)
- *** Broad (br)** – if the Gaussian distribution is abnormally broad (*this is more for describing a bond that spans many energies)

Exact transmittance values are rarely recorded

So let me as well to give you some more idea you know it is important to note that peak intensities actually are 10 to be effects of the three factors one if the peak intensity is very strong let me speak is very tall and absorption is highest as mentioned slow medium ones which peak is mid height that is not very tall and not by small also so ways in which these transmission is very small one a week and that means transmission is very high.

(Refer Slide Time: 34:46)



So as I if I go back to this plot I can show you there this is a week this is tall and some cases you can see medium height here so all these three scans the signals are available everywhere sorry and broad you can brawl then the Gaussian distribution is abnormally brought this means actually more the descending bond that spans have more energies exact as median values are really recorded here.

So that is why although we can apply the beers law but it is not you know good to use the exact attachments to get good results or the quantity results from that okay so what else the infrared spectroscopy can do.

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Capabilities of Infrared Analysis

- ❖ Identification and quantitation of organic solid, liquid or gas samples.
- ❖ Analysis of powders, solids, gels, emulsions, pastes, pure liquids and solutions, polymers, pure and mixed gases.
- ❖ Infrared used for research, methods development, quality control and quality assurance applications.
- ❖ Samples range in size from single fibers only 20 microns in length to atmospheric pollution studies involving large areas.

It can actually identify and quantify organic solid liquid gases it can analyze powders solid gels emulsions paste even the pure liquids or solutions polymers and even pure and mixed gases so that means it can analyze everything solid liquid gas so that is why the versatility of this technique.

So important it can be used for all transmission activities like quality control quality assurance even nowadays we actually have a scientist to use to detect different kinds of bonds presence samples sizes can be single fibers like only 20 microns in lengths given atmospheric pollutants nowadays people do lot of studied atmospheric pollutants.

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Applications of Infrared Analysis

- ❖ Pharmaceutical research
- ❖ Forensic investigations
- ❖ Polymer analysis
- ❖ Lubricant formulation and fuel additives
- ❖ Foods research
- ❖ Quality assurance and control
- ❖ Environmental and water quality analysis methods
- ❖ Biochemical and biomedical research
- ❖ Coatings and surfactants
- ❖ Etc.

So which can be large not only that it can be used in pharmaceutical research forensic investigations polymeric analysis which have showed you lubricant formulations and fuel additives lubricants which are used nowadays many for the many applications and the machine industry can be studied fuel additives you know in different fuels you add different kind of additives.

And whether they are stable in the fuel conditions can be studied that by this way food research is extensively used because food use slot of different kinds of spices where this can be used their chemical sexually while the a student's which I have told you already elemental pollutions and the water pollutions can be studied by this way not only that biochemical research biomedical research can be done coatings surfactants can be studied they all even either polymeric or even metallic or the ceramic materials many others.

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infrared spectroscopy

II. Infrared Group Analysis

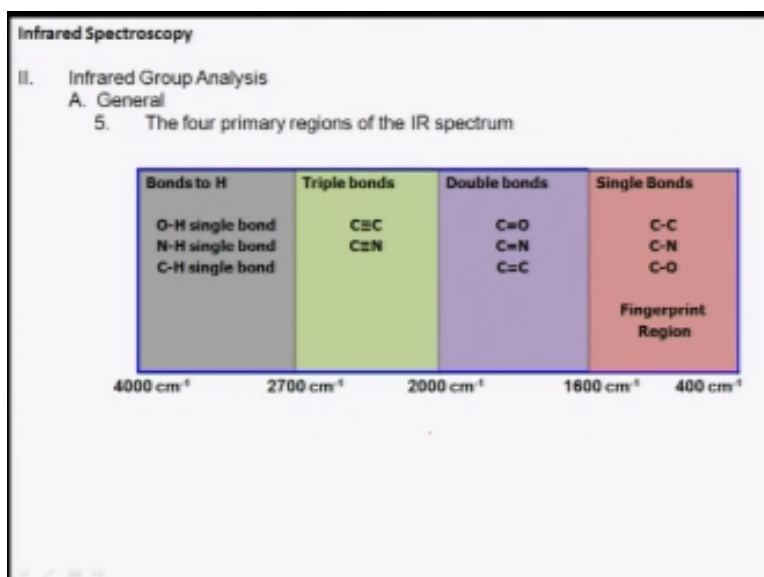
A. General

1. The primary use of the IR spectrometer is to **detect functional groups**
2. Because the IR looks at the interaction of the EM spectrum with actual bonds, it provides a unique qualitative probe into the functionality of a molecule, as functional groups are merely different configurations of different types of bonds
3. Since most "types" of bonds in covalent molecules have roughly the same energy, i.e., C=C and C=O bonds, C-H and N-H bonds they show up in similar regions of the IR spectrum
4. Remember all organic functional groups are made of multiple bonds and therefore show up as multiple IR bands (peaks)

Most importantly they are used in the polymers for to give you all these things in nutshell that in general the primary use of a spectroscopy detect the functional groups but it can be used because it leaves you interaction of the electromagnetic spectrum with axial bonds it can provide a quality probe of the functionality of the molecule because it can actually give different configurations it can actually give you different conversion molecules present in the more in the image.

Because one molecule can straight spend our maybe you can have different kind of positions are the energy levels so that can be detected seen most types of the bonds and covalent molecules have roughly the same energies like CC double bond or co double bonds or choc NH single bonds they swap in similar regions of the IEEE spectrum and you must remember that all the organic functional groups are made of multiple bonds therefore show up in the multiplier bands that so you seem a pan that many picas are there in one bands.

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And in general so we can actually determine for regions h NH see a single bonds they follow in this range tippie bouncy CCN acetylene and the other tributes carbon-hydrogen bonds two thousand five seven hundred two thousand double bonds false 2002 1611 angel so that is here that is you know and our co they commonly finger petitions so that is why we use these techniques to dream it all kinds of bonds you.

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