## Spectroscopic Techniques For Pharmaceutical & Biopharmaceutical Industries Prof. Shashank Deep Department Of Chemistry, Indian Iinstitute of Technology Delhi Lecture 3 Introduction to Spectroscopy 3

Hello students. Welcome to the third lecture of this course. We will continue to discuss basics of the spectroscopy. So in the last lecture we discussed at electromagnetic radiation can behave as both wave and particles. So it has dual character. Similarly, we looked at the materials and what we found out is that small molecules a small particles can act as a very small part can act as wave, right?

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So in this lecture, what we are going to discuss is about colour of the molecules, one colour of the different objects and we know that nature around us is colourful. If you look around, you will see objects of different colours.

For example is cherries are red. and blueberries are blue. So we need to understand why cherry looks red or blueberry looks blue.

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So similarly, if you look at the stars in the night, some of them will look great and some of them they look blue. Now questions why? So scientist during early days also were anxious to know the answer of this. Anxious to know the answer of this.

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As such, light itself has no inheriting colour. So our perception off this different colour is due to the interaction of light with the matter, their accent of light with the matter. So the colour which we perceive is basically due to interaction of light, which has no inherent colour with the matter the matter. (Refer Slide Time: 2:52)



So The way electromagnetic radiation can interact is with matter in many forms. So if radiation falls on a matter, what can happen is a part of it can be absorbed, part of it can be absorbed. Most of them can be observed after absorption. What can happen is that material, well reemit the electromagnetic radiation and this process is called Emission.

The second thing which can happen is that once a part of flighty Gerson job, the rest of them will get transmitted, rest of them can get transmitted. Again. The third scenario is that after interaction of EMR with matter, the electromagnetic radiation can get reflected, can get reflected and you are flexing is when the angle of incident, with normal is equal to this angle, this angle, then electromagnetic radiation falls on the matter It can undergo the fraction.

It means it can undergo bending, it can undergo bending and the be a scattered light, can be a scattered by matter and scattering can be in all that direction scattering can be in all direction.

So this is five most common way, in which electromagnetic radiation interacts with matter so it can get absorbed, it can emit the absorb light after the up absorption, a apart of light can get transmitted electromagnetic radiation and can get reflected. It can undergo the fraction or it can undergo a scattering.

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So what is colour? Colour of an object we see is due to wavelengths that reach our eyes reflected, transmitted and muted or scattered. So the colour which we perceive it due to the wavelength of the light, which reaches our eyes, either due to reflection, due to transmission due to emission, or due to scattering.

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Our eye acts as an optical instrument they are sensitive to visible part of the electromagnetic radiation. So from wavelength of 380 nanometre to 710 nanometre A wavelength of light which we receive is perceived as colour.

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Now eye has different parts. eye has different parts. You have cornea, Iris and Lens. This is vitreous humor and there is a retina and this is your optical nerve. These are the few parts of our eye.

As Other optical instruments require. eye has an maze forming surface and this is called cornea. This is called cornea and he also have a detector which is basically retina this the yellow one is your retina.

Now, so the is photosensitivity tissue and this retina has two types of receptor rods and cones. You can see here these are the rods and these three are cones. Rods are numerous and adapted to low intensity light and that's why they are better suited for the night vision, but Rhodopsin which is contained in rod cells bleaches it rapidly in the bright light and so rods are not active and the presents of light. (Refer Slide Time: 8:16)



On the other hand, cones are suited for daylight vision and concept, different kind of colour mass. They have three colour pigments here you can see these two are blue, these two are green, and these two are red.

So most humans have three colour pigment. That may not be true with the animals or other species, but humans has three colour of pigments. Some of human may have two colour pigments and that may lead to your colour-blindness.

So when light falls on a particular wavelength falls Wavelength on our eye can stimulate these three cones to different extent and depending on percentage stimulation and these cones or you can perceive the colour of an object and this can be from this region to this.

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So what I mean by this is when you see a leaf, it looks green. Now what is the reason for it being green is when electromagnetic radiation for example, from sun falls on a leave it to reflect green colour or light of green light of green wavelength.

When it reaches our eyes, that different cones associated with a different concepts associated with the retina gets stimulated to different extent. For example, when green light reaches our eye, the green cones are stimulated to 90% and similarly a bit off-rate cones are also stimulated and when it happens you see a green colour, you see a green colour.

So based on percentage or based on extent of his stimulation of these three cones we see colour or we see object of different colour. So in this case it is the reflective light which reaches our eye. (Refer Slide Time: 10:59)



Here we see the leaf green. Since when light interacts with leave, a green part of it is reflected to our eyes and that is the reason why leaf looks great.

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Now you must have seen the rays from sun or rays from a electric bulb. So this is basically part of what we know as emission spectrum. So what happens is that if you look at the light coming from Sun, they are example of continuous a spectrum.

So here we are looking at emitted light. We are looking at emitted light, emitted light can be of different types. One is continuous spectrum, which is because of continuous spectrum which means that you are, which your Sun is emitting.

The radiation of all colours. similarly, your electric ball does same thing and when you receive light off every Wavelength, then you know that you are looking at continuous as spectrum.

On the other hand, if you look at the Lens, for example, zinc lamp and rubidium lamp or mercury sulphide lamp you will see different colour. They are a emitting they are emitting wavelength of , a particular colour

So here and listen is not a collection of every wavelength but one wavelength or a very narrow range of (())(13:17), similarly, if you look at the led lights, led lights, they also emits, they also emit light of a certain wavelength and this kind of source are example of source for discreet spectrum.

Discrete means particular wavelength Discrete means your emission of a particular web. Whereas continuous spectrum means you are looking at looking at a light which is a combination of almost every wavelength almost everywhere.

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Colour of an object can be due to abortion and transmission can we do to have jobs on and transmission. So a gem. This particular gem looks red because it transmit the red colour it transmit the red colour. So when incident light or light incident on a this kind of gem, it transmits only that it colour and that is why it looks red.

Other colours are absorbed, other colours are absorbed, the colour can also be due to scattered light. So for example, from the sunlight, we get a continuous spectrum. What does that mean is they are eating the waves of whole range of wavelength from the sun.

When sunlight passes through atmosphere, there are several particles in the atmosphere and what they do is they scatter wavelengths or scatter waves of different wavelengths and we observe different wavelengths. Scattered to different extent are scattered to different extent and that's why some of them may reach out by some of them may not reach our eye.

A particular wavelength if suppose, a wave of blue wavelength, or suppose blue light reaches our eye. So then we will see object as blue. I will see the sky as blue. So during the different part of the day, during the different part of the day, the sun or, the sky will look different because we are receiving the light or receiving a different kind of light, different kind of light during different friend of the day.



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For example, the atmospheric scatters blue light more effectively then red light hence, mostly blue light reaches our eyes when we look at this guy. So during the daytime, that light, the blue light is scattered more effectively than red light and since during that daytime it is the scattered light, which reaches our eye and so we see sky blue.

So here is the yard your scattering. Shown by shown in the figure and you can look that blue is a scattered more where is red, is a scattered less and the blue one, reaches is our I during the day time that is why during the daytime sky looks.

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On the other hand, if you look at the sun or a sky, when sun is setting or when sun is rising, what will happen is you are not looking at the scattered light or you can tell it is not the scattered light, which is reaching our eye.

It is unscattered light, which is reaching our eye and so during the sunset or sunrise, Sun looked red again. The atmosphere scatters blue light more effectively than red light. Hence during the sunset unscattared light reaches our eye. and that's why your sun looks red. Or your sky looks red.

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So this is about why we perceive a particular colour of an object. For example, apple is red blueberries are blue. This is because the light which is reaching our eye is not a light. itself it is a light which is reflected, reflected, transmitted, or scattered by an object.

So we can utilize this or what we can do is, instead of eye we can observe Wavelength frequency. I've jog and muted, transmuted or scattered by an object at a molecule. By placing our detector in the appropriate direction, what we will get is spectrum so instead of eye Wavelength frequency absorb, emitted transmitted or scattered by an object at a molecule can be observed by placing our detector in the appropriate direction (Refer Slide Time: 20:29)



So what I mean by that is, so suppose we are going to look at transmitter light in that case what do we need to do is if you want to see to a transmitted light. What we can do is you can put our detector in the line with light source. and sample and in this line itself you put a detector , then you can look at that transmitter light.

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You can look at the transmitter, like but if you want to look at emitted light. What we need is that do is that if you take this line between light source and sample, you need to put your detector perpendicular to this line, perpendicular to this line. So by putting detectors at appropriate place, you can see the transmitter light or ammeter light.

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Type of S	Spectroscopy
Absorption Spectroscopy	Transmission Spectroscopy
Emission Spectroscopy	Reflection spectroscopy
Refraction spectroscopy	Scattering spectroscopy
Diffraction spectroscopy	Optical rotation Spectroscopy
	ce spectroscopy

So based on the interaction, interaction between electromagnetic radiation and object, you can think of different type of spectroscopy absorption spectroscopy transmission spectroscopy emission spectroscopy reflection spectroscopy refraction spectroscopy scattering spectroscopy Diffraction is spectroscopy, optical rotation Spectroscopy or interference spectroscopy So several kind of a spectroscope is posse. Several kinds of spectroscopy is possible depending on the interaction of your electromagnetic radiation with an object Each of this spectroscopy can give you and give you a particular kind of information and if you combine the information from different kind of spectroscopy you can completely analyse a particular sample or completely analyse a particular sample

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Now next topic is quantization of energy and this is very important concept in the spectroscope.

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So if you look at the spectrum observed from different sources, particularly emission spectrum, you will either see a continuous, a spectrum in which radiation is distributed over all frequency, not just a few, a specific frequency ranges. So you can see it is going from the red to blue. So basically radiation is t is distributed over all frequency in continuous spectrum. For example, if you see the emitted light from a sun it is an example of a continuous.

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So then we get continuous spectrum when we heat a body or any hard body produces a continuum spectrum. So if it is hot enough, it will look like something like this. So you are seeing from violet to violet to light of every frequency light of every frequency and digitally how it will look like is this.

So this is your intensity versus wavelength and you can see that at every Wavelength you can see intensity, it may be low intensity, high intensity, but at every wavelength or light emitted consists of everywhere and that kind of spectrum is called continuous suspect. (Refer Slide Time: 24:52)



In the line spectrum. Now you can see that there are lines you don't see the light of every wavelength. So when you can see this kind of a spectra, so pattern of brightest spectral, lines is generally produced by an element. So an element will show pattern of. If you hit an element and you can see pattern of brightest spectral line and that is known as lines Spectra.

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Line Spectra			
<ul> <li>Any gas to which energy is applied, either as heat or a high voltage, will produce an emission line spectrum like this</li> </ul>			
'or digitally like this			

So when you can see Line spectrum, one is by hitting and eliminate another by applying heat to a guys applying heat to a gas. And that will produce an emission Line spectrum like this where you can see at only this only light of this particular wavelength is absorbed if you like to see it digitally, how does it look like? This will look like this. So you can see intensity is you can see intensity at some particular weapon, some particular weapon not at every, not at every level.

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And so there are two different kinds of things which I already talk. And show you and emission lines, one is your gases. When they are heated was so the emission lines similarly when you hit elements, you will see emission lines sunlight and interesting thing about emission lines line of an element is every element has different lines. Spectrum or they emit, light of different web lands.

And this can be used to know whether a particular element exists in the sample or not. So for example, the hydrogen with, show you this kind of spectrum, whereas sodium, will so you this kind of a spectrum with different element had different emission lines and that can be used as finger print to detect the atoms or elements.

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What are, what is the absorption spectroscopy? So absorption spectroscopy is basically pattern of dark spectral lines where light within a range of narrow frequency ranges has been removed narrow frequency ranges has been removed.

So we looked at two kinds of emission spectroscopy. Now this is your absorption is spectroscopy. What is happening here is light or particular wavelength is getting absorbed and that is why those lines are light of those frequency has been removed from the light

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And when we can see that any gas placed between a continuous spectrum and the observer, well produce a absorption line spectrum like this. So for example, if you place a gas, we're doing sun and us, you can see the have absorption line spectrum. And absorption line spectrum, looks like this. And digitally it will look like this. So you can see that the line here, the light is missing, light is missing. So light of this particular wavelength are missing because they are absorbed by the sample.

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So if you look at atomic and molecular spectra, absorption and emission of electromagnetic radiation by atoms or molecules occur only at discrete energy value. So if you look at the Line spectrum, you will see that only emission is happening of electromagnetic radiation off only discrete energy value or emission is of particular wavelength. t not emission is not like the emission from the sun.

Similarly, if you look at absorption Spectra, absorption Spectra of a gas, you will only see that absorption is happening of particular wavelength. Part of that mean is that absorption emission of electromagnetic radiation.

Occur only at discrete energy value and classical physics one predict that it will predict absorption or in the sun at, all energy levels of all energies. And so what we have seen that at emission spectra, particularly in line Spectra, if you take a hot gas, it will. Show you line emission spectra and if you take a light and you passed through coal gas what you look at absorption spectra.

In both these cases, Line spectrum and absorption spectrum the absorption and emission happens at discrete energy values So emission happens or this value emission happens or this value emission happens and this value, not all the values. Similarly, absorption happens at this value absorption happens at this value, these two values, this and this, not at all values. And that can not be explained by classical physics.

This observation can be explained only on the basis of quantization of matter So what I'm going to discuss now how the science about quantization of energy formed.

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So people started to study the black body radiation first we, should know what is a black body a black body is a theoretical or Model body, which all radiation and falling on it, reflecting or transmuting none.

So whatever falls on this it absorbs everyone absorbs waves of every wave length It does not transmit Anything. This is also an object which is perfect emitter of radiation over all wavelengths So it is your perfect absorber it is perfecting emitter (Refer Slide Time: 33:08)



A hot body emits a electromagnetic radiation, varying frequency. Depending on the nature of object and it is temperature, as a temperature increases in a peak wavelength emitted by the black body decreases.

What are that mean is if the increase in the temperature the emission will be off higher frequency and emission by the black body will be of higher frequency light, as the temperature increases. The total energy also increases what does that means is not only frequency is increasing with the temperature the energy of emitted light is also increase. So as temperature increases both energy and frequency of emitted light increases. (Refer Slide Time: 34:11)



So this is called Planck spectrum. Here we will show you. Now look at this that when you hit an object at 300 k they are not showing any colour because it doesn't fall in their visible light A thousand K it regress to glow deep red and you can see that this part of this frequency, you can see it overlapping with the or reason red region at 4000 K, the maxima is a red and so it becomes very hot at 4,000 feet you can see maximize you and if you go to 7,000 k Maxima covers all this wavelength in the visible region and that is why it looks white hot So as object is heated radius and it emits peaks at higher and higher frequency, higher and higher frequency

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And an opaque object, emits electromagnetic radius and according to temperature, if you heat a iron rod, if it is hot enough it will first glow deep red like this if you hit more it will glow as a reddish orange. And if you heat make it even hotter, then it will glow like a yellowish white.

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Similarly, if you look at the sky in the night-time it was show stars of different colour and that is because that is because of it's temperature. So red stars are relatively cool. Yeah. Yellow stars such as our sun is hotter and a blue star is very hot. So red star temperature is around 3000 degrees Celsius and yellow star like our sun is 6,000 degrees Celsius and a blue white star is at 40,000 degrees Celsius. So because of temperature, because your temperature, a particular star will look red or blue. So it is the temperature which decides colour of the stars.

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Now let us understand this, what is happening. We know that our atoms are in motion and everything is composed of atoms which are constantly in motion. The hotter the object, the faster the average motion of atoms. If you compare between a hotter object and cooler object, a hotter objects in the hotter objects,

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The molecules are in faster motion as their atom two motion Collisions gives of energy and the energy and emitted as light.

So the hotter the object, the faster the average item and more energetic they have just collision faster that the more there are and your emitted light will be of higher energy.

So as you increase the temperature motion between a motion of items, increases, there are more collisions and the light and emitted is of higher frequency. Light emitted is of higher frequency.

So the more energetic the average collision is bluer, the average light that is given now since e is equal to (())(38:36).

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Now more colleagues in that occurred, the more light that is given off per surface area So this explains you why that increase in temperature, both frequency and intensity of the emitted light increases.

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So two things. hotter is bluer and hotter is brighter. These are the observed phenomena from black body radiation So people tried to explain this in terms of several laws and there are three very important laws which are used to explain this phenomena.

One is Planck's law, blackbody, radiation, the second Wien' displacement law and third is Stefan Boltzmann Law.

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So first attempt or good attempt was made by Rayleigh Jean's law. They calculated an energy density per unit frequency and according to this law this energy density is given by this expressing 8 pie mu square by c cube and average value of (())(40:01) and according to classical physics, this average value of e is equal to 80 average value of e is 80.

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When you applied this classical physics, what you will get is this kind of prediction. So radiation, the energy of radiation versus wavelength so of look like this. If classical physics was true, what classical physics predicts that event relatively cool objects. Should radiate in UV and visible region and in fact classical physics predicts that there will be no darkness.

But that is not true. Now observed one is this one that if you, so this is your increasing wavelength and if you go in this direction you have increasing frequency. So with the increasing frequency, you can see here that it goes initially up and then it goes down and that this quite the different from the curve explained on the classical physics. This difference is known as the ultra violet catastrophe.

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That difference in the experimental and the curve obtained based on your classical physics was explained by Max Planck. Max Planck explain this. The deviation by assuming that they energies of the oscillations of electrons which give rise to the radiation must be proportional to integral multiple of the frequency E equal to n h mu.

This recognition that energy change energy changes in discreet quanta at atomic level mark, the beginning of quantum mechanics and Plank won the Nobel prize in physics in 1918.

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So what were the blank concept at average per mode or quantum, is the energy of quantum time, the probability it will be a occupy and the value of E is now no longer required to KT. It basically divided by exponential h mu by kt minus 1.and when he used this formula, he was able to predict the experimental, or able to explain the experimental observation, experimental observation.

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Now Wien's displacement law, this law tells about how temperature affect the F maximum of frequency of the P on the Emission maximum either as the temperature of body increases the wavelength at the emission peak decreases and frequency emission (())(43:26) increases and there is basically the proportionality relation between frequency and temperature, frequency and number frequency and that is known as Wien's displacement law

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Stefan Boltzmann Law talk about intensity, that total energy emitted is proportional to temperature power 4 So the black body radiation curve shape is explained by the shape of black body radiation is explained by Planck's law.

The temperature dependent on a frequency dependent on temperature is explained by the your Wien's Displacement Law and energy dependence on temperature You explain by Stefan Boltzmann law

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Intensity at all wavelength increases at the temperature of black body increases and your the total energy being radiated increase rapidly at the temperature in places we have seen that (())(44:39) Law works for lower frequency but it diverges at higher frequency and divergence for higher frequency is called the ultraviolet catastrophe. We already discussed that these things

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Now the next of the observation of important the heat capacity of Mono atomic solids. Classical physics predicts a constant value of 25 joules per Calvin per mole for the molar heat capacity of monarch atomic Solids.

Whereas when we do experiment at low temperature, what we will observe that molar heat capacity approaches 0. So here is a plot between Cv by 3 and K and KT by (())(45:32). Classical physics predict that CV by 3 in case should have value of 1.

But when you do experiments at higher temperature when KT by e is high, the classical physics prediction is right, but at low temperature it fails at low temperature fails. In fact, heat capacity of monoatomic solid approaches 0 at low temperature. This experimental observation can, again, be explain based on planks theory, assumption of discrete energy value again led to a model that match the experimental observation, experimental observation.

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So based on the explanation for black body radiation and molar heat capacity, also the discrete spectrum observed in case of your, in case of atoms, late to the concept of quantization of energy.

So in the blackbody radiation we saw how we can explain the ultra violet catastrophe by taking discrete value of energy. Similarly, molar heat capacity of monoatomic Gases at low temperature. Can be explained by, can be explained by taking or discrete value of energy levels.

Similarly transition between atoms can also be explained, or emission a spectrum of atom can also be explained on the discrete value of your discrete value of energy discrete value of energy.

If suppose there are discreet value of energy level, then you can explain emission or absorption emission, emission or absorbs of particular wavelength if suppose this to energy level exist, then if there is absorption, it will absorb wavelength corresponding to this Delta e value and the relationship between Delta e and lambda is given by this. If there is emission from this level to this level, then again you can see the emission of the Wavelength corresponding to this Delta E.

And if suppose the energy differences higher, then lambda will be smaller. If the energy difference is your smaller than lambda will be higher. So on absorption of light of energy delta e spaces go to higher energy level and if there is a discrete value this delta e will be fixed and you will get or your sample is absorbed, sample will absorb lambda of this wavelength.

So in this relation H is Planck's constant mu is frequency, C is velocity of light and lambda is wavelength of light. So in this lecture we have discussed about quantize on off energy and concept of quantization of energy. is important because this because this quantization of energy led to development of quantum chemistry and which is quantum chemistry is quite important to understand the basics of spectroscopy So I will stop here and thank you for listening.

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I will like to acknowledge this books which I am referring regularly to make slides and I have taken lot of figures animation from the (())(50:13) sources and I have tried to acknowledge them and please let us know if there is omission and thank you again for listening. I will see you in the next lecture. Thank you. Bye.