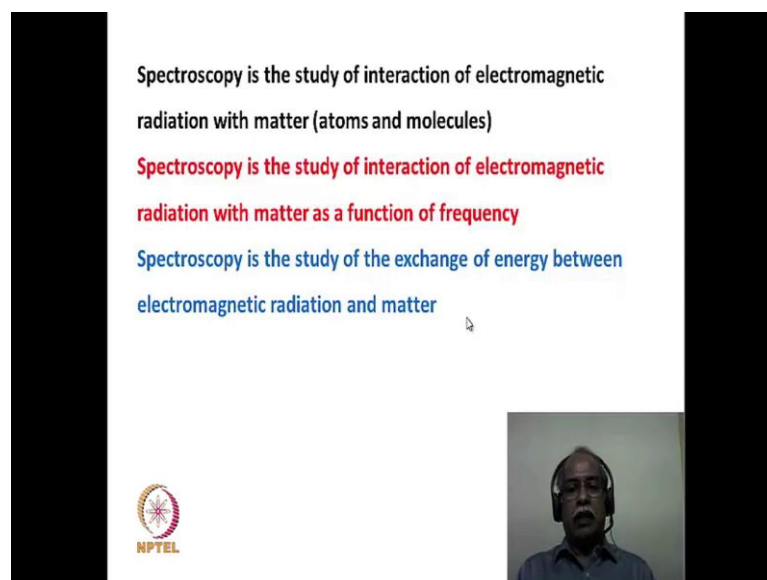


**Application of Spectroscopic Methods in
Molecular Structure Determination
Prof. S. Sankararaman
Department of Chemistry
Indian Institute of Technology, Madras**

**Lecture – 01
Application of Spectroscopic Methods in
Molecular Structure Determination**

Hello, welcome to module 1 of the course on Application of Spectroscopic Methods in Molecular Structure Determination. In this module, you will ask questions about what is spectroscopy? What is a spectrum? What is electromagnetic radiation? What are the various regions of the electromagnetic radiations and when matter is interacting with electromagnetic radiation? What are the changes that take place in the matter? What is a nature of light? What is absorbance? What is transmission? All these terminologies that are used in spectroscopy, we will deal with in this general module in this particular presentation.



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Spectroscopy is the study of interaction of electromagnetic radiation with matter (atoms and molecules)

Spectroscopy is the study of interaction of electromagnetic radiation with matter as a function of frequency

Spectroscopy is the study of the exchange of energy between electromagnetic radiation and matter

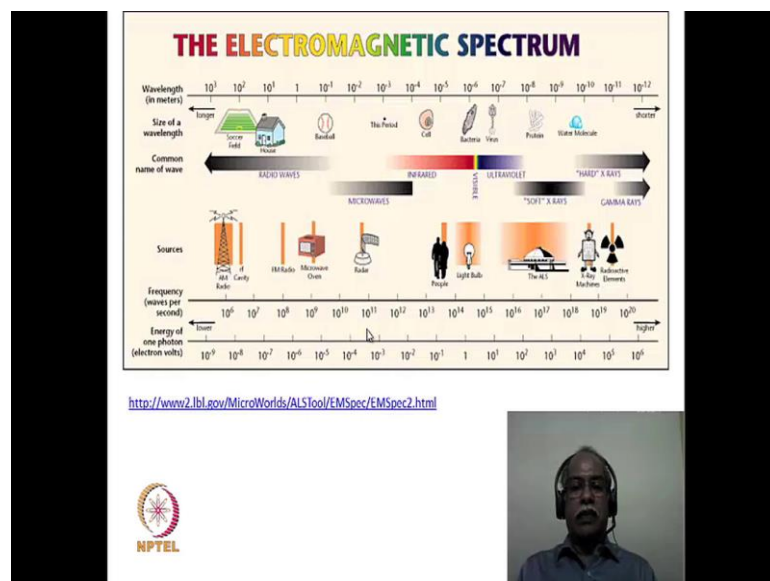
 

Now, spectroscopy in the broadest term is defined as the study of interaction of electromagnetic radiation with matter and when we talk about matter we are dealing with atoms and molecules. So, essentially the interaction of atoms and molecules with

electromagnetic radiation is what constitutes the term spectroscopy. Spectroscopy is a study of interaction of electromagnetic radiations with matter as a function of frequency because whenever we record a spectrum, we are essentially scanning various frequencies and recording the response of the material that we study for the various frequencies of the electromagnetic radiation. Spectroscopy is the study of the exchange of energy between electromagnetic radiation and matter.

Here, we are talking about the electromagnetic radiation being the source of energy the energy of the photon of the electromagnetic radiation gets transferred on to the atoms and molecule and the changes that occur in the atoms and molecule as result of the absorption of energy is what is recorded as a spectrum.

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Here is an electromagnetic spectrum dealing with various frequencies and various energies of the photons and the different regions of electromagnetic spectrum. The regions of the electromagnetic spectrum are labeled here as radio waves, micro waves, infrared waves, visible region of the electromagnetic spectrum, ultraviolet region of the electromagnetic spectrum, the soft and the hard x-rays. Finally, the most powerful energetic gamma rays in the right-hand side of the spectrum. Now, the top scale corresponds to wavelength which is expressed in meters which is a unit of length. Just to

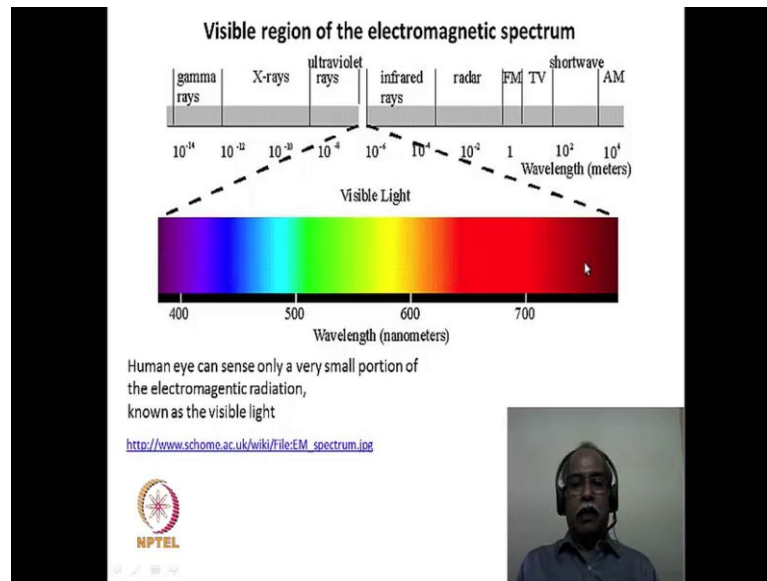
understand what is this unit of length actually means in terms of the dimensions of commonly seen objects, we can for example; correlate the wavelength of radio frequency region corresponding to something like 10 meters to about 1000 meters corresponding to the size of a building or size of a stadium and so on.

On the other hand, if you look at the size of a molecule which is of the order of a pico meter or so. We are talking about the dimensions of the wavelength of the x-rays or the gamma rays in this particular region. Suppose, if we take a tiny dot on a piece of paper which corresponds to about a millimeter or less than a millimeter that corresponds to the micro wave radiation region of the electromagnetic spectrum. So, just sort of gives you a perspective of what this unit of dimension in terms of the length unit corresponds to commonly absorbed objects on our day to day life. In the bottom, the frequency scale is mentioned. Frequency units are waves per seconds, in other words per second is the unit that is normally used for the frequency scale. As you can see here the frequencies starts from 10^6 to the power 6 per second to about 10^{20} per second in the highest frequency region which is a gamma ray region. As the frequency increases the energy content also increases because frequency is directly proportional to energy in terms of $E = h\nu$, where $h\nu$ is the frequency of the electromagnetic radiation.

The last scale corresponds to energy per photon of the electromagnetic region, spectral regions. For example, we are talking about something like 10^{-9} electron volt. Electron volt is the energy unit that in which this is this particular scale is expressed 10^{-9} corresponds about to a nano electron volt is what we are talking about a very low energy in terms of the energy content of a photon of a radio frequency wave. On the other hand, if you come to the gamma rays it is about 10^6 one mega electro volt is what we are talking about and this is a high energy radiation, normally we call it as ionizing radiation because they ionized substances through which they pass through.

So, we have a wide range of energy content per photon of the various regions of the electromagnetic radiation depending upon what kind of a radiation that is being used. Different processes take place in atoms and molecules and the response of the atom and molecules for the various frequency regions is what is recorded as a spectra.

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In the electromagnetic spectrum, there is a very small portion what is known as the visible portion of the electromagnetic radiation and this is a only portion to which human eye is sensitive. In other words, we will be able to perceive only the colors of this particular region and not see the colors or not see the other regions like for example, the ultraviolet or the infrared spectroscopy. They are invisible to the human eye, human eye is sensitive to only about 380 or 319 nanometer, which is the violet region of the electromagnetic spectrum to about 760 or 780 nanometers, which is the red region of the electromagnetic spectrum. This is very important to know because when we talk about the UV visible spectroscopy, you will be dealing with this particular spectral region in the UV visible spectroscopic technique.

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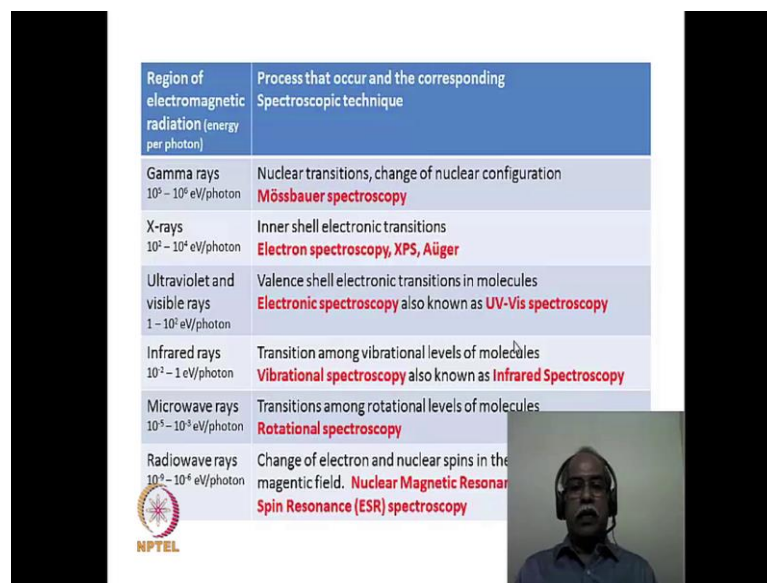
Spectroscopy is the study of interaction of electromagnetic radiation with matter (atoms and molecules)

Depending on the region of the electromagnetic spectrum used for the excitation, different processes occur in atoms and molecules leading to different spectroscopic techniques



Having defined the spectroscopy as a study of interaction of electromagnetic radiation with matter, now we have to depending upon the region of the electromagnetic spectrum that is used, what are the various processes that can take place in atoms and molecule? How does one receive information in these processes? And what are the spectroscopic techniques that corresponds to various wavelength regions of the electromagnetic spectrum?

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Region of electromagnetic radiation (energy per photon)	Process that occur and the corresponding Spectroscopic technique
Gamma rays $10^2 - 10^6$ eV/photon	Nuclear transitions, change of nuclear configuration Mössbauer spectroscopy
X-rays $10^2 - 10^4$ eV/photon	Inner shell electronic transitions Electron spectroscopy, XPS, Auger
Ultraviolet and visible rays $1 - 10^2$ eV/photon	Valence shell electronic transitions in molecules Electronic spectroscopy also known as UV-Vis spectroscopy
Infrared rays $10^2 - 1$ eV/photon	Transition among vibrational levels of molecules Vibrational spectroscopy also known as Infrared Spectroscopy
Microwave rays $10^2 - 10^3$ eV/photon	Transitions among rotational levels of molecules Rotational spectroscopy
Radiowave rays $10^2 - 10^6$ eV/photon	Change of electron and nuclear spins in the magnetic field. Nuclear Magnetic Resonance Spin Resonance (ESR) spectroscopy

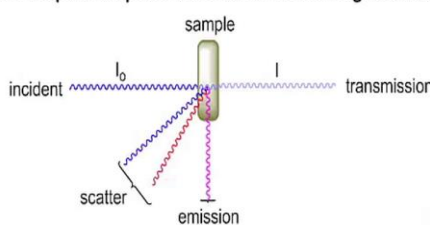
This is actually defined in this particular table. If you look at column number one, the region of the electromagnetic radiation, energy per photon is given starting from gamma rays which are the powerful rays to the radio waves which are the least energetic rays that we are dealing with in this particular table. Now, the processes that occur in molecules and atoms corresponding to this particular energy regime is what is mentioned on this particular column and the spectroscopic technique, corresponding spectroscopic techniques are also given in red. Now, if we take for example, gamma rays, gamma rays are very powerful high energy photons and they can cause transitions within the nucleus causing the change of nuclear configuration and this essentially constitutes the Mossbauer spectroscopy.

On the other hand, if we come to microwave which are very, very low energy radiation the transition among the rotational levels of a molecule is what is happening in the case of absorption of the microwave radiation and this essentially constitutes the rotational spectroscopy of the electromagnetic spectrum corresponding to the microwave radiation is called the rotational spectroscopy. Now, if we talk about radio wave frequency region of the electromagnetic radiation then we are talking about change in the nuclear or the electron spin in the presence of the external magnetic field. In the presence of an external magnetic field, nuclear spins and electron spins have different energies, ground state and

excited state and the cause of spin change from the ground state to the excited state is what is normally absorbed during the electron and the nuclear spin resonance electron spectroscopy. NMR and ESR are the techniques which are responsible for this and we will deal with NMR in this particular spectroscopic course in much more detail.

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Types of responses upon interaction of electromagnetic radiation



The diagram illustrates the interaction of electromagnetic radiation with a sample. Incident radiation with intensity I_0 enters from the left. Upon hitting the sample, it is partially transmitted as radiation with intensity I on the right. Some radiation is scattered away from the sample, and some is emitted from the sample.


I_0 is incident intensity of the radiation and I is transmitted intensity

The ratio I/I_0 is known as transmittance (T)

$\log (I_0/I)$ is known as absorbance (A)

Types of spectroscopic techniques:

- Absorption spectroscopy (e.g. IR)
- Emission spectroscopy (e.g. fluorescence)
- Scattering spectroscopy (e.g. Raman)



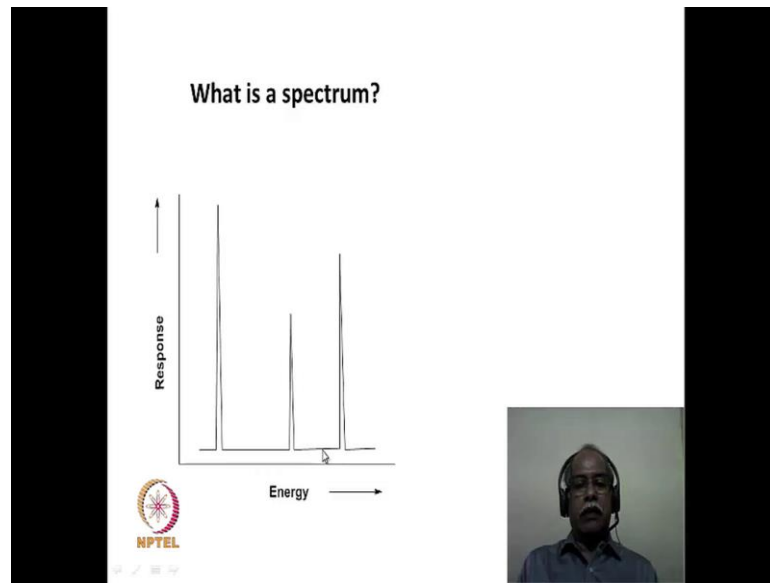
This particular slide tells us something about the responses upon interaction of electromagnetic radiation. In other words, when a sample is being excited by electromagnetic radiation, what are the processes that can occur in the sample? Now, let us consider an incident light falling on the sample in this particular direction. I_0 is the intensity of the incident light that is falling on this substance. The substance can absorb certain amount this light and then transmit the remaining light into the other side, I is the intensity of the transmitted light.

Let us say for example, so I_0 minus I would correspond to the absorbance or the intensity that is being absorbed by the sample itself. Instead of absorbing the light the sample can simply scatter the light for example, if it is scatters the light and if it is the light of the same wavelength then we call it as Rayleigh scattering. If it scatters light of different wavelength, then we call it as a Raman scattering. Raman spectroscopy is based on the scattering phenomena and we deal with Raman spectroscopy along with our

vibrational spectroscopy for the structural residential purposes. Now, instead of the absorbed energy instead of being scattered and so on, the molecule can also emit light for example, in the form of light emission which corresponds to the emission spectroscopy. We have fluorescence spectroscopy and phosphorus spectroscopy as emission spectroscopic techniques corresponding to this. Now, let us define certain terminologies that are used in the area of spectroscopy. The ratio of I by I_0 , in other words the intensity of transmitted light to the intensity of the initial light is what is known as the transmittance or capital t is the symbol that is used for this particular terminology.

Now, logarithm scale of I_0 divided by I is what is known as the absorbance, capital a is what is used for us the symbol for this particular term and absorbance transmittance are related to each other as you can see for example, one is the logarithmic quantity which is logarithm of 1 by T is what is known as the absorbance. Now, the type of spectroscopic techniques that one can have depends on the kind of phenomena that one observes. If the absorbance of the light is what is being observed, then we call it as Absorption spectroscopy. If emission is what is observed, then we call it as the emission spectroscopy. If scattering is what is being observed then we call it as scattering spectroscopy, examples of Absorption spectroscopy are the infrared, UV visible spectroscopy, rotational spectroscopy and so on. Emission spectroscopy corresponds to fluorescence and phosphorous and spectroscopy and scattering spectroscopy for example, corresponds to Raman spectroscopy.

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Now, let us ask this question what is a spectrum? A spectrum is essentially a plot of energy in the x-axis and the response that is being received from the sample as y-axis. The energy is the energy of the electromagnetic radiation that is being applied in this particular case and the response is the kind of response that one records in terms of whether it is an absorbance or transmittance or emission intensity or scattering intensity. What is being recorded on the y-axis and the peaks that are normally seen in the spectrum are essentially due to the intensities of absorption or transmittance or intensities of emission or scattering is what is plotted against the energy of the electromagnetic radiation.

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Beer Lambert law – a quantitative correlation

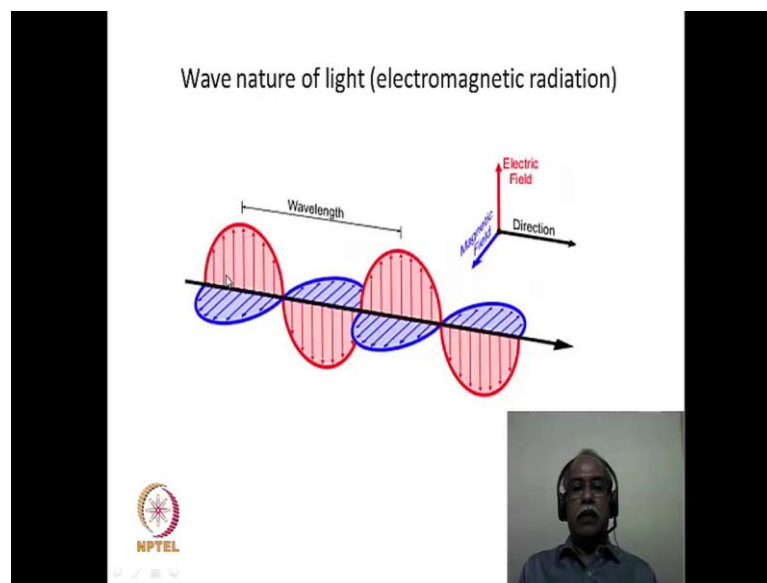
Absorbance = $\log(I_0/I) = \epsilon c l$

ϵ = extinction coefficient / molar absorptivity
 c = concentration of substance in mol L⁻¹
 l = path length in cm



Certain laws are governing the quantitative aspects of spectroscopy is important to understand. One is called the Beer Lambert law is a very basic law dealing with the quantitative correlation between absorbance and the concentration. Now, this expression is what is known as the Beer Lambert law, absorbance which is actually logarithmic ratio of I_0 by I is directly proportional to the concentration. In other words, when light is passing through a medium it depends on how many number of molecules that it encounters, absorbance will be accordingly more or less. In other words, absorbance is directly proportional to the number of molecules the light interacts on it is path. Now, the proportionality constant is what is known as extinction coefficient or the molar absorptivity and extinction coefficient or the molar absorptivity is a constant at a given wavelength for a given substance and this is what makes the absorption spectroscopy a quantitative tool in order to find concentration of unknown substances.

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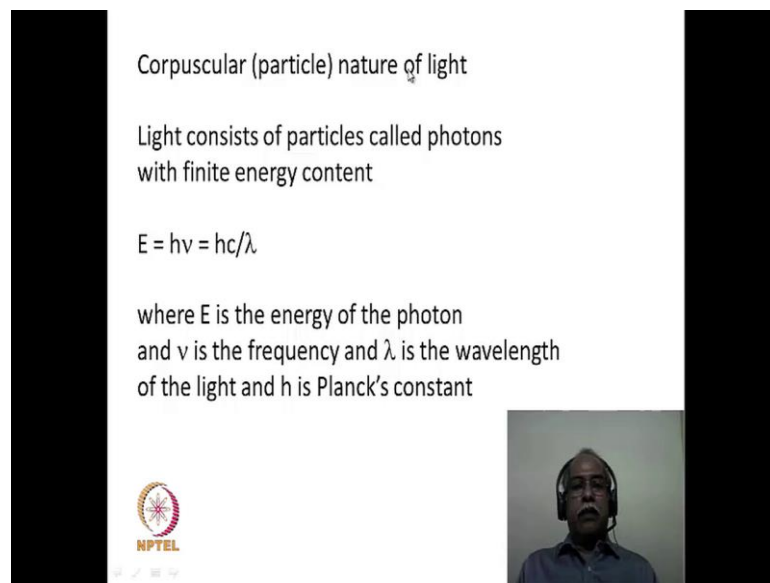


Now, let us have a look at the nature of light. Light can be described to have dual nature that is both the nature of wave as well as particle. In the wave nature of light, it is actually explained in the form of this particle diagram that is shown here. If x is the direction of propagation of the light then we can define two fields, one is an electric field another one is the magnetic field. The blue one is the magnetic field and the red one is the electric field. Thus, you can see here the two fields, namely the electric field and magnetic field lie orthogonal to each other. In other words, they are perpendicular to each other and light can be expressed in the form of a sine wave consisting of two sine waves interacting sine waves for example, one corresponding to the electric field, the other one corresponding to the magnetic field.

The distance between the hump to the hump is what is known as the Wavelength and this wavelength is what we referred in terms of the electromagnetic spectrum that earlier we saw in terms of the defining the regions of the electromagnetic spectrum with the different Wavelengths and the arrows that are shown here are the vectors of the intensity or the amplitude of the electric field in this particular case. The amplitude of the magnetic field is shown in the blue color. So, this is essentially the wave nature of light is being explained in this particular manner and whenever molecules interact with electromagnetic radiation in spectroscopy like for example, a electronic spectroscopy or

infrared spectroscopy or rotational spectroscopy it is supposed to be the electric field that is interacting with the molecules in those kinds of spectroscopy. Unlike for example, in the case of magnetic resonance spectroscopy it supposed to be the magnetic field that is interacting with the magnetic nuclei. So, it is in the case of NMR and ESR essentially the magnetic field is what is interacting with the molecules.

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Corpuscular (particle) nature of light

Light consists of particles called photons with finite energy content

$$E = hv = hc/\lambda$$

where E is the energy of the photon and ν is the frequency and λ is the wavelength of the light and h is Planck's constant

NPTEL

In order to explain the other nature namely the corpuscular nature of the light one proposes that light consists of particles called photons with finite energy content. In other words, e is equal to h nu this is very famous expression which deals with the energy of photon which corresponds to the h which is the Planck's constant and nu the frequency of the electromagnetic radiation, which is correlated to the velocity of light in vacuum namely c for example, divided by lambda. In other words, e is equal to h nu which is equal to the h c by lambda, where lambda is the wavelength of the light that we are dealing with.

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Calculation of amount of energy per photon

$$E = hv = hc/\lambda$$

Consider light of 500 nm wavelength, per photon energy is

$$E = \frac{6.626 \times 10^{-34} \text{ J s} \times 3.0 \times 10^8 \text{ m s}^{-1}}{500 \times 10^{-9} \text{ m}}$$
$$= 3.98 \times 10^{-19} \text{ J}$$

Light of 297 nm corresponds to 400 kJ mol⁻¹



In order to calculate the amount of energy that is present in a photon and one can use this expression very easily. Let us have an example of how much of a photon energy is present in a 500-nanometer wavelength region which is the visible wavelength region for example. So, all you have to do is plug in the Planck's constant which is available readily which is 6.626 into 10 to the power minus 34 joules per second and put in the value of the velocity of the light which is about approximately 3 into 10 to the power 8 meters per second divided by 500 nanometers, which is 500 10 to the power minus 9 meters.

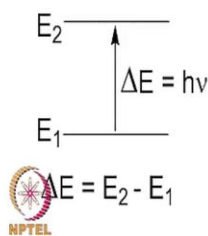
Now, the units which are the time units they cancel out each other. The distance unit namely the meters they cancel each other finally, you are ending up with the energy which is joules in this particular case. So, the energy content of a photon of a 500-nanometer wavelength light is about 3.98 10 to the power minus 19. Light of 297 nanometers which is in the ultraviolet region has much higher energy. In fact, this is about 400 kilo joules per mole. This is per mole is what is expressed, in other words, if you want to convert per photon energy into a per mole energy you have to multiple this quantity by per photon quantity by avogadro number which is 6.023 into 10 to the power 23. So, if you multiply the per photon energy by avogadro number you get the energy per mole of the corresponding wavelength.

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Energy levels are quantized

There is a finite energy gap between the ground state and excited states of a molecule

When the energy of the incident photon matches with this energy difference absorption takes place




E_2

E_1

$\Delta E = h\nu$

$\Delta E = E_2 - E_1$

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Now, according to the quantum mechanics, energy levels are quantized. We are talking about electronic energy levels or vibration energy levels or rotational energy levels they are quantized. What is meant by quantization? The energy gap between the ground state and the excited state is a finite one. When we say it is a finite one then, the energy difference when the energy of the incident photon matches with the energy difference ground state and the excited state one can expect the absorption of the light to take place. In other words, E_1 let us say ground state energy and E_2 is the excited state energy of certain system it could be a electronic energy or it could be vibrational energy or it could be rotational energy as the case may be. Now, the difference in the energy is ΔE and the ΔE is equal to $h\nu$. So, when the ν corresponds the electromagnetic radiation of certain frequency corresponds to the difference in the energy between the ground state and excited state, absorption is going to take place.



Otherwise, if there is a different frequency which does not match this particular criterion of ΔE , then the absorption will not take place that is what is implied in this particular diagram.

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The population ratio of the two energy levels is governed by Maxwell-Boltzmann distribution

$$\frac{n_2}{n_1} = \exp[-(E_2 - E_1)/kT] = \exp(-\Delta E/kT)$$

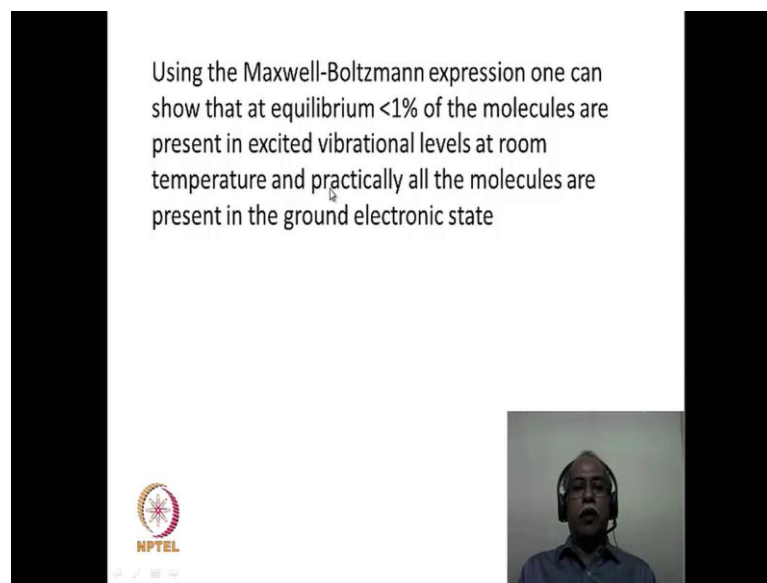
n_2/n_1 is ratio of number of molecules in excited state to the number in the ground state



Now, once you say there are two energy levels, there should be a population in this energy level of molecules and there should be a population in this energy level in this molecule. One can easily calculate the difference in the population or the ratio of the population in the excited state to the ground state using the Maxwell-Boltzmann distribution. Maxwell-Boltzmann distribution is expressed by this particular equation here, n_2/n_1 is the ratio of the number of molecules in the excited state n_2 , n_1 is the number of molecules in the ground state and this ratio corresponds to the ΔE divided by kT in terms of exponential term being added here. Now, in the Boltzmann distribution one can calculate the ratio of the excited state to the ground state using this particular equation.

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Using the Maxwell-Boltzmann expression one can show that at equilibrium <1% of the molecules are present in excited vibrational levels at room temperature and practically all the molecules are present in the ground electronic state



The image shows a presentation slide with a white background and black text. The text reads: "Using the Maxwell-Boltzmann expression one can show that at equilibrium <1% of the molecules are present in excited vibrational levels at room temperature and practically all the molecules are present in the ground electronic state". In the bottom right corner of the slide, there is a small video feed of a man wearing glasses and a headset, speaking. To the left of the video feed, there is a logo for NPTEL (National Programme on Technology Enhanced Learning), which consists of a circular emblem with a star-like pattern and the text "NPTEL" below it.



When you do that using the Maxwell-Boltzmann distribution expression, one can show that at equilibrium we are talking about thermal equilibrium. Let us say at room temperature less than one percent of the molecules are present in the excited state vibrational level at room temperature that is we are talking about the vibrational spectroscopy. When we say there is a ground state vibration and in the excited vibration state. Nearly 99.9 percent of the molecules do exist in the lower vibrational level, compared to the higher vibrational level and when we come to electronic energy states when we talk about ground state electronic state to the excited state electronic state because electronic states have much higher energy gap practically all the molecules will be present in the ground state compare to the excited state and this is very important to understand because this kind of population difference is directly responsible for the sensitivity of the technique that we are talking about.

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As far as electron (ESR) and nuclear spin (NMR) states are considered only ppm levels of excess population exists in the ground state, the ground state and excited states are nearly equally populated at thermal equilibrium

This is due to the very small energy difference between the spin states

This has important consequence on the sensitivity of the various spectroscopic techniques

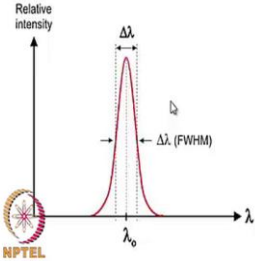


Now, let us look at the NMR spectroscopy or ESR spectroscopy, where we are talking about nuclear spin state, ground state and excited state. The energy difference between the two states are extremely small compared to the energy states of the electronic spectroscopy or the infrared spectroscopy. So, as a result of that the population difference is extremely low only parts per million difference is present in the population difference is present between the ground state and the excited state and that makes the NMR spectroscopy as the least sensitive spectroscopy techniques that one can think of compare to for example, the electronic spectroscopy or the vibrational spectroscopic technique. So, the population difference is directly responsible for the sensitivity because the intensity of absorption is directly proportional to the excess population that is present in the ground state in comparison to the excited state. So, when the entire population is in the ground state this spectroscopic technique will be very sensitive because we have a large number of molecules to excite from the ground state to excited state.

On the other hand when you have already reached equal population between the excited state and the ground state there is very little excess population present in the ground state to be excited to the higher level. So, accordingly the intensity of absorption will be low. So, the sensitivity will be consequently low in the case of NMR and other spectroscopy techniques.

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Natural spectral line width
Although energy levels are quantized, absorption and emission does not occur at one precise frequency; it has measurable width known as natural line width. It is defined as full-width at half-maximum (FWHM)



Now, let us define another parameter what is known as the natural spectral line width. Let us say, if the energy levels are quantized then the absorption and the emission should occur in a precise frequency. In other words, a monochromatic frequency is what would be responsible for each absorption and emission wavelengths that we are talking about, but usually this does not happen. There is a measurable width to any spectral line which is known as the natural line width of the spectroscopy and this is defined as shown in this particular diagram. This is essentially a lambda plotted against the relative intensity you can see that the spectral line has a particular shape usually at Gaussian shape and the if we take half the intensity and measure the width of the spectral line here, this is what is known as the full-width half-maximum spectral width and this is what is normally known as the natural spectral line width.

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The finite life time of the excited state and the consequent uncertainty in the excited state energy gives a finite width to spectral lines, due to the Uncertainty principle

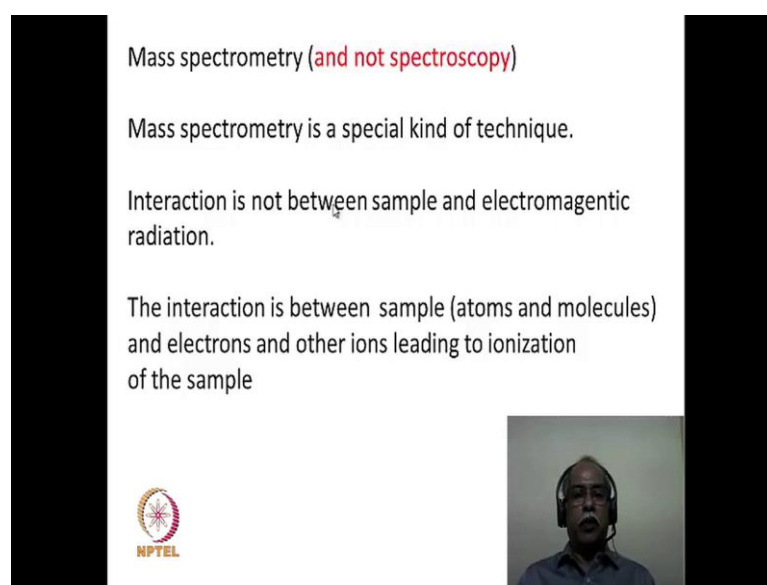
$$\Delta E \cdot \tau \geq h/2\pi$$


Now, why do we have a natural spectral line width instead of simply line kind of a spectrum? The finite lifetime of the excited state is what is responsible for the line width. In other words, the finite lifetime of the excited state and the consequent uncertainty in the excited state energy is what gives the line space for many of the spectroscopic techniques. Now, the uncertainty principle is expressed in a different format in this particular case. Normally, uncertainty principle is expressed in terms of momentum and position where you can have either uncertainty in the momentum or uncertainty in position. In this particular case, this is expressed as the energy and lifetime in other words this is could be the uncertainty in the difference in the energies or uncertainty in the energy and this will be the lifetime of the system.

Now, when we talk about for example, lifetimes of the excited state or the relaxation times, if you are talking about ultraviolet spectroscopy for example, the relaxation times are the typically of the order of the peco seconds or faster. So, there is a large uncertainty associated with a excited state energy level and this uncertainty in the excited state energy level is what causes the line broadening which leads to the natural line width of the UV visible spectroscopy. On the other hand, if you look at NMR spectroscopy, where the relaxation times of the order of the seconds much slower than the relaxation times of the electronic spectroscopy, the uncertainty in the energy of the excited spin state is very,

very low as the result of that you get sharp peaks less than one hertz width natural line width what we get in the case of NMR spectroscopy. Now, so far we have been talking about spectroscopic technique which have some commonality in terms of either being absorbance or the emission kind of a spectroscopy, where electromagnetic radiation is used as a source of energy for causing certain types of transitions. It could be electronic transition, it could be spin transition or it could be vibrational transition and so on. The commonality of all the spectroscopic that we talked about is very different when we compare it with for example, Mass spectrometry.

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Mass spectrometry (and not spectroscopy)

Mass spectrometry is a special kind of technique.

Interaction is not between sample and electromagnetic radiation.

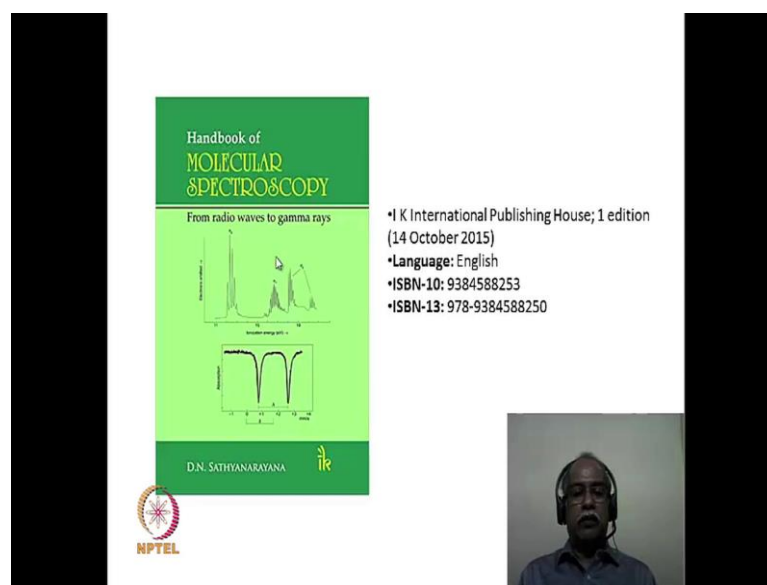
The interaction is between sample (atoms and molecules) and electrons and other ions leading to ionization of the sample



First of all mass spectrometry is not a spectroscopic technique at all. It is a spectrometry technique there is no interaction between electromagnetic radiation and sample in mass spectrometry, is a very special kind of technique. It is an extremely useful technique for molecular structure determination that is why it is normally put under the spectroscopy many spectroscopy books talk about mass spectrometry as well because it is useful in structural elucidation problems. In mass spectrometry, we are talking about interaction between a sample that is an atom or molecule and an electron which is usually high energy electron of the order of 70 electron volts or 100 electrons volts, leading to ionization of the sample fragmentation of the sample and so on. We will deal with the mass spectrometry slightly later and just wanted to bring out the difference between the

various spectroscopy and mass spectrometry in terms of the, this spectroscopy being spectrometry being a special case and it comes under the spectroscopy essentially because of it is useful not because of it is commonality with the other spectroscopic methods.

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Now, let us see what are the resources that we need to follow this particular program. At least one or more books need to be referred to. This book which was published last year that is in 2015 by Prof. D. N. Sathyanarayana, who was a former professor in the Department of Inorganic and Physical Chemistry in Indian Institute of Science, Bangalore. This is a very nice book, it deals with various spectroscopic techniques right from radio waves to gamma rays for example, in other words he is covering the nearly the entire electromagnetic radiation region in this particular book. It gives very fundamental aspects of the many of the spectroscopic techniques with suitable examples and so on. I would recommend that you read this book for clear understanding of the basics of these spectroscopic.

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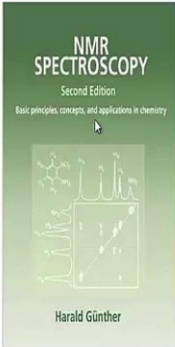


Spectroscopy – 2009
by Donald L. Pavia, Gary M. Lampman, George S. Kriz, James R. Vyvyan
• Cengage Learning (2009)
• Language: English
• ISBN-10: 8131505766
• ISBN-13: 978-8131505762





This is another book by name it is Spectroscopy by Pavia and others. There are four other authors associated with this particular book. This is essentially a spectroscopy book with emphasis on problem solving, in other words structural elucidation problem solving is what is the emphasis that is shown in this spectroscopy book. It is an excellent text book it is available in Indian edition should be possible for some of you to buy this book and refer this particular book.

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NMR Spectroscopy: Basic Principles, Concepts, and Applications in Chemistry, 1995
by [Harald Günther](#)

- Wiley-Blackwell; 2nd Edition edition 1995
- Language: English
- ISBN-10: 047195201X
- ISBN-13: 978-0471952015



NMR Spectroscopy by Herald Gunther is a very famous text book for example, it is very lucidly presented text book in the terms of the concepts and applications of NMR spectroscopy. So, this spectroscopy book is also going to be very useful for this particular course.

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Spectrometric Identification of Organic Compounds
Robert M. Silverstein, Francis X. Webster

- Wiley; Sixth edition (2006)
- Language: English
- ISBN-10: 8126509724
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This particular book namely Spectroscopic Identification of Organic Compounds by Silverstein and Webster is actually used to be Silverstein and Basler. Now, it is called as Silverstein and Webster in terms of the authors names and this is published in 2006. This is also an excellent source of problem solving sessions in the spectroscopy.

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Finally, the Organic Spectroscopy by William Kemp is also a good source of information particularly, if you are dealing with organic structural which we will be doing in this particular course.

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Now, I would like to thank you for patient hearing. We will see you in the next module.

Thank you.