Chemistry II: Introduction to Molecular Spectroscopy
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Lecture - 2
Interaction of Radiation with Matter

Welcome back to the lecture. In this lecture on the Introduction to Molecular Spectroscopy series. We shall look at the introduction of radiation with matter and looking more in detail. But first I would like to impress upon you why we need to study spectroscopy in such detail.

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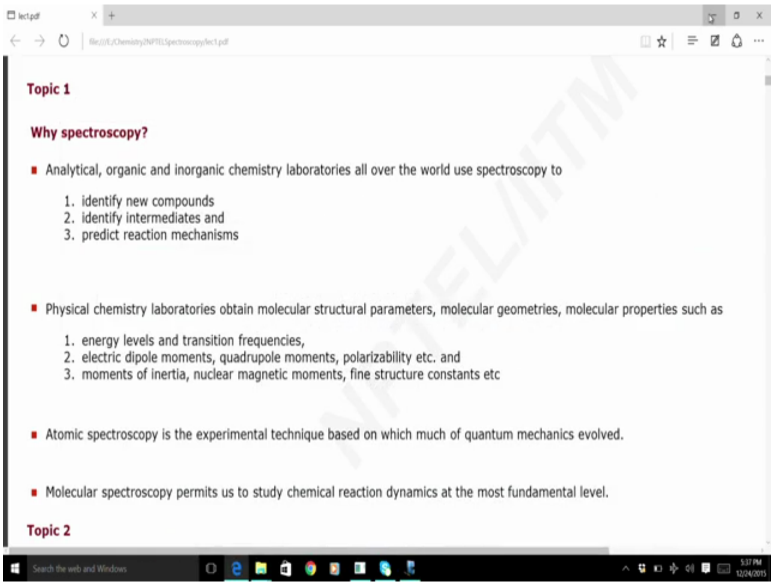

There are many reasons, and I have listed some of these things. Since this is largely text I have the model prepared as a text material. So, why we need to study spectroscopy? Many reasons; first of all spectroscopy is the experimental science for understanding most of the developments of quantum mechanics theories the predictions etcetera at one level. But, from the point of view chemistry spectroscopy is the subject through which we are able to identify and analyze molecules and also new molecular compounds. So, the entire branch is an analytical organic and inorganic chemistry laboratory all over the world. They use spectroscopy for several reasons; obviously to identify new compounds to identify intermediates in chemical reaction, because very often these intermediates are slightly long lift is possible for us to be actually detects them using several spectroscopic techniques depending on life time.

It is also important in our ability to understand how a chemical reaction takes place. Therefore, predicting the reaction mechanism is extremely important objective and in the activity of any chemist, particularly organic in organic chemist. In the physical chemistry laboratories of course they use molecular spectroscopy to obtain signatures of molecules, that is what is a molecule in terms of it is size shape the bond lines bond (Refer Time: 02:20) different elements in the molecule. And therefore, the entire range of molecular structural parameters molecular geometries and molecular properties the electric and magnetic properties of the molecule can also be studies by using spectroscopic techniques as well as the quantum mechanical and physical chemistry theories.

So the energy level of molecules, of course we cannot measure the energy levels, but we can measure the transition of the energy levels in the form of the light that is observed that the light is emitted. Therefore, the transition frequency can be experimentally observed which validate the calculation of the energy levels. We can study molecular electrical properties such as charged distribution in a molecule, if you think about carbon dioxide as an example; carbon dioxide does not have an electrical charged distribution which is polarized, that is the carbon of a center between the two oxygen, the positive and the negative charge center coincide in terms of the electro negativities. And therefore, carbon dioxide is not having electric moments at the most elementary level does not have dipole moments.

On the other hand, if the carbon dioxide molecule during vibration is slightly bend you can see that the carbon oxygen bond may have an electric dipole because, the carbon being slightly passing to the oxygen being slightly negative, there is a charge separation and there is a distance between them. Therefore, the charge times the distance gives you the dipole moments and corresponding the of this side there is a other die pole moments. And this two dipole moments being vectors actually add up to give you a net dipole moments. This is during the process of molecular vibration, therefore it is possible for us to identify electric dipole moments which may not be there but which may appear. That is in the case of a molecule such as carbon dioxide.

On the other hand, if you think about say material chloride CH3CL, you know that the carbon chloride is one of the tetrahedral bonds and the carbon hydrogen is the other three tetrahedral bonds that you have. And therefore, there are net dipole moments in the molecule. And such molecular charged distributions due to the atoms in the molecule or measured in the form of dipole moments and they are measured in the form of quadrupole moments, and also in the field of an experiment electric or magnetic field how this charged distributions rearrange themselves, they polarize themselves in the name what are the polaraziblity factors.

So, molecular electrical or magnetic properties are directly studied by associating the electric or magnetic field of the electromagnetic radiation with such properties, and then determining them the changes that happen and so on. Molecular geometries are fully determined by calculating the moments of inertia, the central mass in molecules, and then the moments of inertia about three mutually perpendicular axis. And then the nuclear magnetic moments of the individual nuclei the fine structure constants, such as the chemical shift and the spin coupling constants eventually come to know of in nuclei magnetic (Refer Time: 05:59) and so on. And there are many fine structures constants. Therefore, physical chemistry is very much concern with determining the entire range of properties and distribution of electrical or magnetic charges in a molecule. Therefore, spectroscopy is very important.

Atomic spectroscopy of course is the experimental method is the experimental technique from which method quantum mechanism involved. Remember need more trying to explain the spectrum of the hydrogen using already known, series of spectral line zone Lyman series, Balmer series, (Refer Time: 06:36) series and so on. And you need more came up with the first idea what is called quantizing the energy of the electron in an atom. And therefore, atomic spectroscopy since then is one of the most important branches for understanding quantum mechanical concepts and also experimentally the behavior of atoms in magnetic and electric fields.

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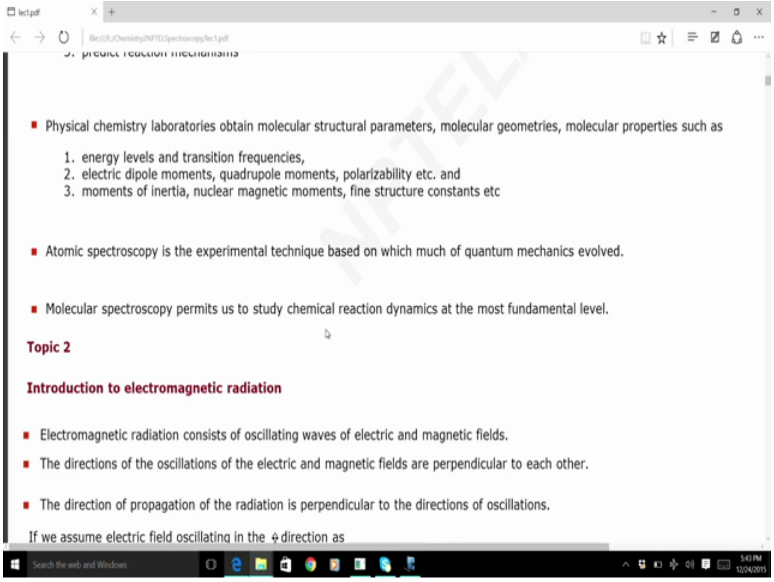

Molecular spectroscopy, of course as to study the chemical reaction dynamics at the most fundamental level and as the atoms move away from a molecule they either (Refer Time: 07:15) from molecule and form other species and so on. If you want to follow that in detail molecular spectroscopy provides you much of the answers. As a field spectroscopy as give you many many answers.

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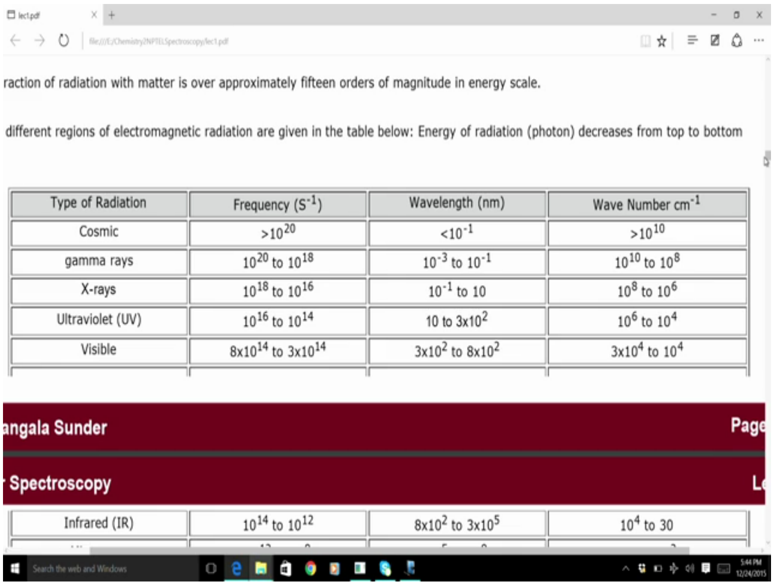

Now it is not all happening in some simple process, it does all of this does not happen by taking the lector magnetic radiation any in which way that you would like to, but understanding the factor different energies, different electromagnetic radiations, different energies have different impacts on the molecule. First of all how do we classify electromagnetic radiation for spectroscopic studies? Here is one small table that you can see that gives you the type of radiations approximately in the corresponding frequency ranges, and also the wave length corresponding to that frequency or the wave number corresponding to that.

Most common unit of wave number is not a meter inverse but centimeter inverse that is what you see in most text books. Of course, wave lengths are often described in manometers or even sometimes in micrometers. Frequencies always in the form of second inverse and therefore it are this unit is known as hertz. Cosmic radiation has a very very high frequency and that for the individual photon as an extremely large energy. Gamma rays have frequency in the range this is the approximate range, in the range between 10 raise to 20 oscillations per second to 10 rise to 18 oscillations per second. And the corresponding wave length which is obtained from the relation by note down in the last lecture, it is approximately 10 to the minus 3 nanometers to that is this is like a (Refer Time: 09:15) meter then 10 to the minus 1 nanometer. And the wave number is about 10 to the 10 to 10 to the 8.

X rays are next lower in energy with a frequency between 10 to the 18 hertz to 10 to the 16 hertz and the wave length is between a nanometer to one tenth of a nanometer. Ultra violet rays are the lower in energy the each photon if you write e is equal to h mu the ultra violet rays as lower energy then the X ray photon. And you see the frequencies 10 to the 16 hertz to the 10 to the 14 hertz and the wave length and wave numbers are accordingly the number you see here.

This is an approximate solution for the energy. And then visible light which are familiar with all of us are impacted by so much actually a very narrow range of electromagnetic radiation frequencies is roughly between 8 and 3 to 10 to the 14 hertz. Therefore, it is a very very narrow range in which you see all this all certain colors and also the range of color visible light and the corresponding wave length and wave numbers are given here. These are important in understanding what properties that they allow us to investigate.

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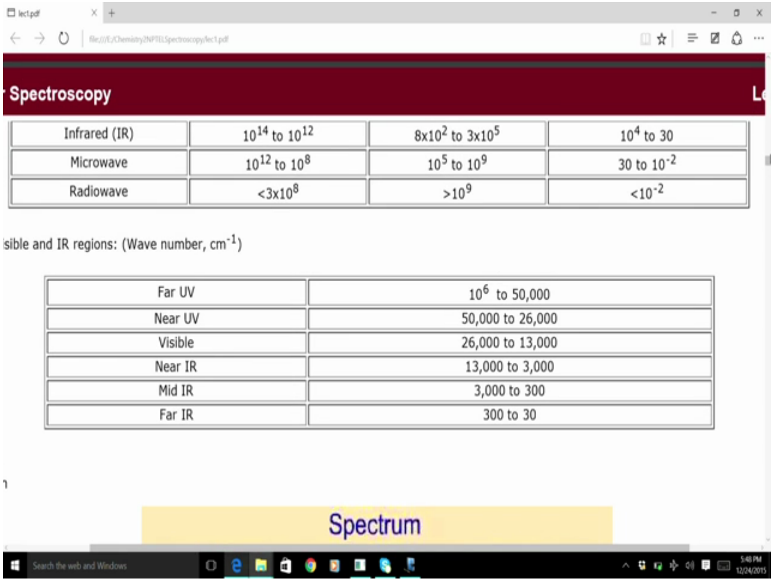

Below visible light or infrared radiation microwave radiation and radio wave both micro wave and radio wave are extremely important in studying magnetic properties of nuclei magnetic properties of the molecule, and therefore in the nuclei magnetic (Refer Time: 10:54) and electron magnetic the energy corresponding to micro waves and radio waves are typically used. You can see that the micro wave frequency is roughly between this is one tenth of a gigahertz, a gigahertz is 9 hertz and this is about a 1000 gigahertz.

So, you can see that this is the range of frequencies and the corresponding wave length and wave numbers are given here. And the radio wave is of course among the lowest in energy with the frequency in less than a gigahertz, it is about a 300 mega hertz that is what you have. And the wave length is 10 to the 9 nanometer, it is almost a meter that is why it is called a radio wave it is a meter wave. So, these are the typical classification of radio electromagnetic radiation.

But in the visible range and the visible and to the UV visible or near visible range, there is further classification of radio electromagnetic radiation for you UV near UV visible near infrared mid infrared and far infrared. And this are approximately corresponding to the different types of interaction that light will have with either the electronic motion or with the nuclear motion or with the overall rotation of molecular. Therefore, this is important to remember, the approximate numbers of the wave numbers are given here.

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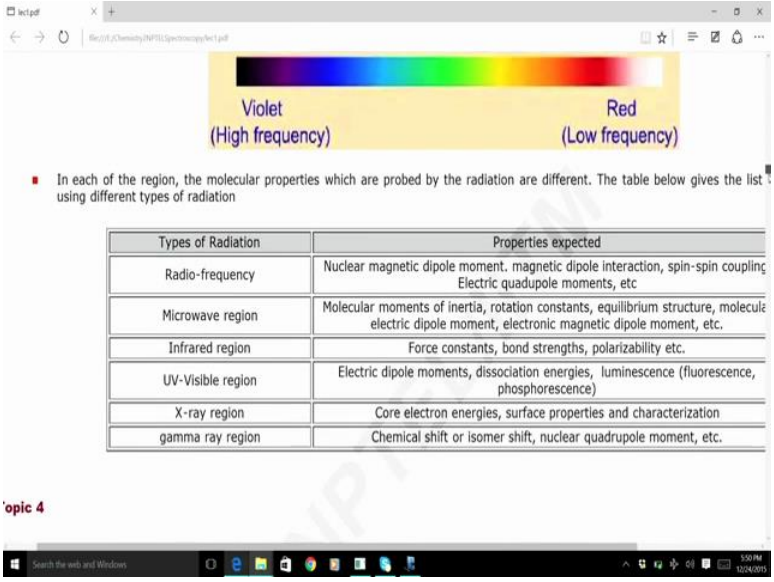

The spectrum, if you look at it the colorful spectrum that you have is actually only for UV which is somewhere around here very high frequency to the far IR which is somewhere here very low frequency. This is the visible spectrum roughly between 8 times 10 to the 14 hertz to 3 times 10 to the 14 hertz. Now why it is important, because each of this region as you see in the radiation from cosmic rays to radio waves the molecular properties which are probed by the radiation are different. What are those properties? You can this list below.

So, radio frequency now we go the other way round, radio frequency is lowest in energy. Radio frequency enables us to measure what are called nuclear magnetic dipole moments and therefore the magnetic dipole interaction between nuclei dipole dipole interactions and also the nuclear spins and how they coupled with each other through scalar and tonsorial interactions. And the electric quadrupole moments which are basically charged distributions inside the nuclei which are non spherical charge distribution that is the nuclei it is not a spherical nuclei, but it slightly distorted. And how these non spherical charged distributions interact with non uniform charged distribution outside due to the electrons and those are called electric quadrupole moments. These are fundamental properties of many nuclei. All nuclei with spin quantum number one or more.

All of this are measured using radio frequency and microwave region, where this basically this is what we called as magnetic (Refer Time: 14:29) spectroscopy. Micro wave of course can also be used to measure the molecular moments of inertia and properties known as rotation constants from which it is possible for us to determine the equilibrium structure of the molecule. And through the equilibrium structure we may also be a able to calculate molecular electric dipole moment and the intensities of the radiation in microwave. Therefore, properties of the molecular structure and the molecular electric charged distribution and the electronic dipole moment all those things are measured using microwave spectroscopy.

Infrared region, allows us to determine the bond strengths and most molecules stable and lots of stable moments. The extent to it is molecules can be polarized by external electric fields distorted and the force constant which are roughly proportional to the bond strength. All this properties can be determined by using infrared region. The UV visible region allows us to understand electronic transition in an atom in the molecule. Therefore, the electric dipole moments of due to the electric motion and the dissociation energies of the molecule of what energy are required to break the molecule into dual components etcetera. And also the visible optical properties that we make use of in today life, the luminescence properties that you see here the fluorescence property that you see here.

The phosphorescence property the screen for example, is phosphors therefore those kind of electrical properties are studied using UV visible electromagnetic radiation. X-ray region allows to understand; the core electron energies inside the molecule in an atom. For example, if you have say sodium atom you know from the elementary electronic structure there it as one balance electron and as 10 core electrons which are in the (Refer Time: 16:36) transitions between them can be studies using X ray region because these are very high energies. And also X-ray is extremely important for surface properties and surface analysis particularly in solids and crystalline materials and so on. So, surface properties and characterization are very very useful done using X-ray spectroscopy and gamma ray region which is due to the gamma ray. Gamma rays which are extremely high in energy allow us to study the nuclear properties which are nuclear quadrupole moment and the chemical shift or isomer shift that we need to know.

So, these are some of the properties which are scaled by different radiations of energies. And therefore, you can see that electromagnetic spectrum with a 15 or magnitude in energies between say 20 hertz for the cosmic rays to about a mega hertz 10 to the 6 hertz in the case of the l m r; the nuclear magnetic resonance. The 15 hertz of magnitude scale the entire molecular properties, and therefore it is very important for us to understand each and every one of them in detail.

Of course, this course will give an over view of some of this in the case of micro wave, infrared and electromagnetic spectroscopy. I will not be dealing with magnetic resonance in this particular course, but in a separate course I will give you more details. We will continue this to understand a little bit more about what are the features that we look for in a spectrum in the next lecture.

Thank you.