Introductory Quantum Mechanics and Spectroscopy

Prof. Mangala Sunder Krishna
Department of Chemistry
Indian Institute of Technology, Madras

Lecture - 08
Part – I
Introduction to Molecular Spectroscopy
Why Spectroscopy?

In this set of lectures, we will look at molecular spectroscopy which is an important discipline for Chemistry, Physics, Biology, Biophysics and practically all of science. It is also one of the most fundamental subjects in the sense that, atomic spectroscopy and molecular spectroscopy are the experimental basis from which many of principles of quantum mechanics evolved. In the chemistry laboratories, spectroscopy is an extremely important technique, there is not one single technique of spectroscopy. In fact, it is of such a wide range that we can have detection techniques or spectroscopic techniques from radio wave frequencies to X rays and even higher in energy. We will see as we go along, what are the different type of spectroscopy why we need to do that and so, on

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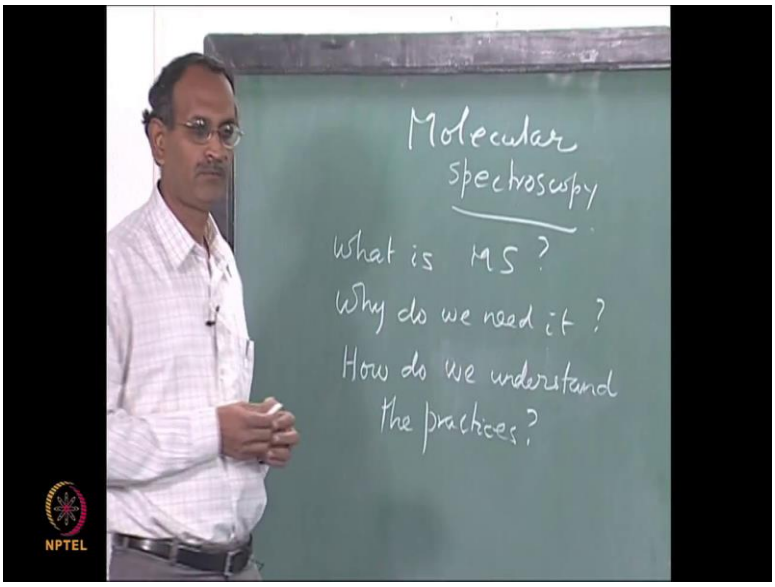

So, we will first look at molecular spectroscopy. What is spectroscopy, molecular spectroscopy why do we need it, and how do the how do we understand the practices. Let us of course, the most important series of questions that one should ask, in understanding this and this is not a pretence and we will answer all of them convincingly

to everybody is not possible because it is of such a wide range. In this series of lectures we are going to look at only the most elementary aspects of molecular spectroscopy. What exactly is meant by molecular spectroscopy? The simple answer is that, it is interaction of electromagnetic radiation with matter. That is the broad definition for molecular spectroscopy or even spectroscopy as a whole and when you talk about the matter, if you restrict your attention to molecules then, you talk about this particular branch of spectroscopy. When you talk about the electromagnetic radiation it of course, has a very, very wide range of frequencies. We recall from the previous learning that you had that, classically one thinks of electromagnetic radiation as a wave quantum mechanically, electromagnetic radiation or after Einstein discovered in 1905 through his interpretation of the photo electric effect that electromagnetic radiation consists of photons there are these two interpretations. We will use the idea for most of our lectures the interpretations that electromagnetic radiation is a wave. It consists of oscillations in electric fields, oscillations of electric fields, oscillation of magnetic fields, perpendicular to the directions of the electric field and both perpendicular to the direction of propagation of light. It is interaction of the electric component of radiation with the electric properties of molecule or interaction of the magnetic component of radiation with the magnetic properties of matter, which determine what we observe in molecular spectroscopy. So, let me go back to some of the slides.

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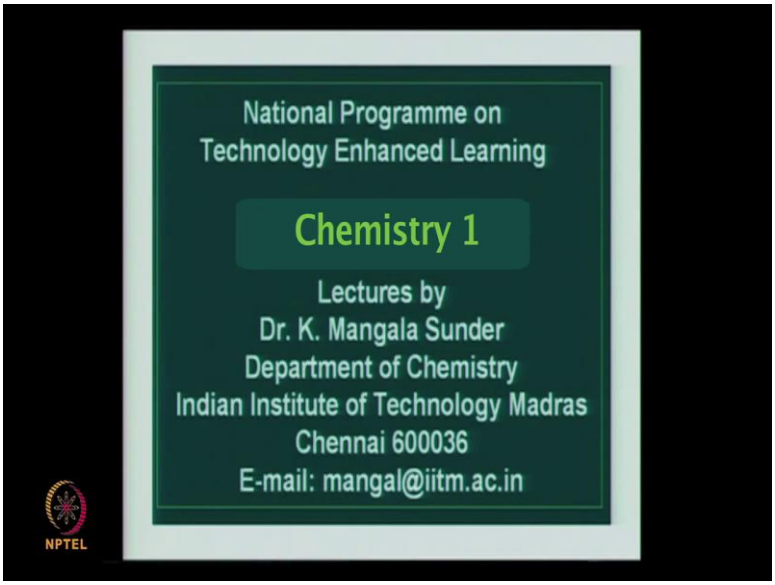

We will see them these questions quantified.

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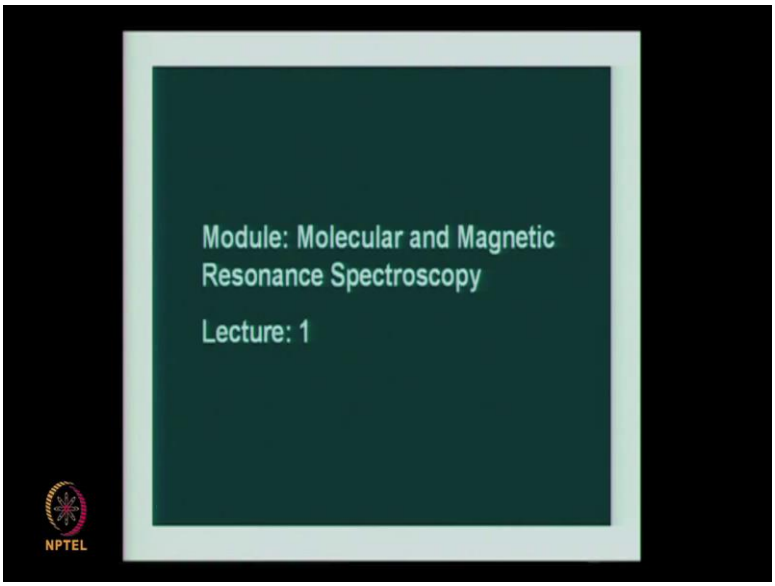

This module will consist of several lectures.

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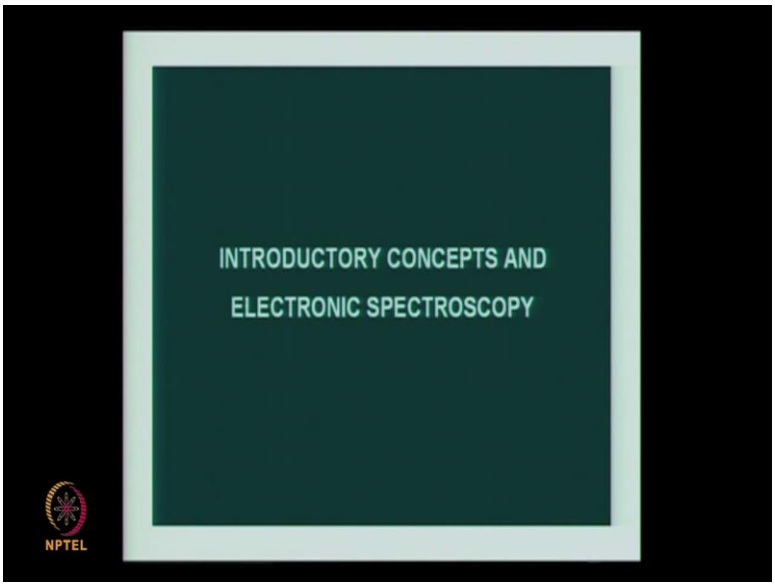

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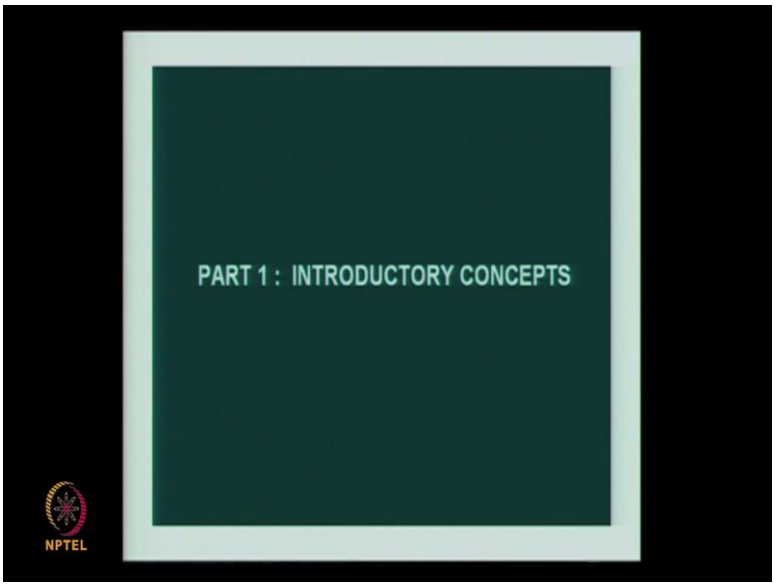

Initially, we will look at the introductory concepts. If time permits, this lecture will continue on to electronics spectroscopy otherwise this will be done in a later lecture.

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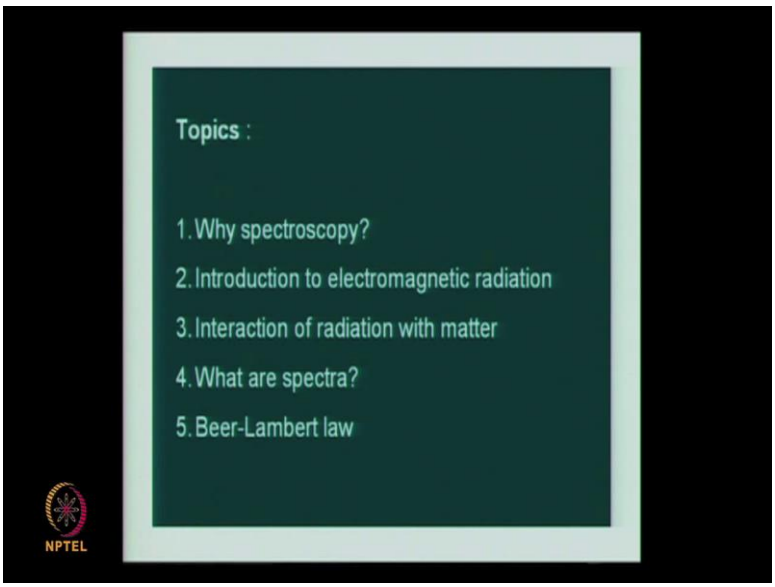

Let us see what are the things that we asked so far why do we study spectroscopy. Let us look at the properties of the electromagnetic radiation in terms of the electric and magnetic field oscillations and what we mean by the interaction of radiation with matter and what do we mean by spectra. Some of the basic terminologies we will clear in this lecture. One quantitative law that most of you should be familiar with when you study

spectroscopy particularly, visible spectroscopy is a well known law in chemistry known as the Beer-Lambert law, we will also show a little about of what that law means. Why do we need to study spectroscopy as a chemist or as a physicist or even as an engineer. The reason for the study of the spectroscopy is the of course, this is what throws light on what matter is. Most laboratories if you think of analytical laboratories, organic chemistry laboratories, the medical labs, the bio labs that you think about.

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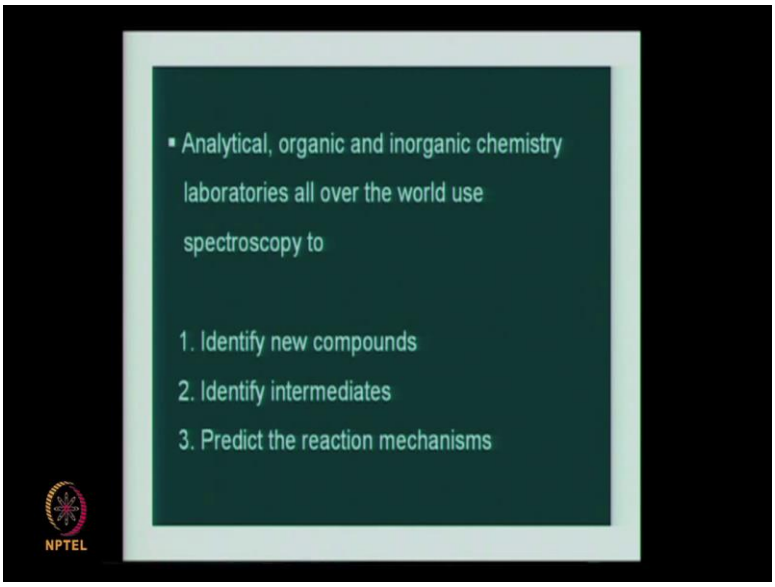

Whatever lab you go to, you see that they use one or the other spectroscopic techniques to do the following; Identify possibly new compounds if they are research laboratories in what we synthesis, to identify some intermediate species, if in a reaction some intermediate species are important and if they are stable an analysis and the study of the intermediate tell us how to make specific synthesis and so, on. So, it is used for us to, as a technique to identify whether the new compounds or intermediates. And of course, many, many chemical laboratories use this in research labs to predict to the reaction mechanisms of various chemical reactions. And these are important for us to understand why molecules behave the way do, and how to make the best use of these reaction properties to benefit of the man kind

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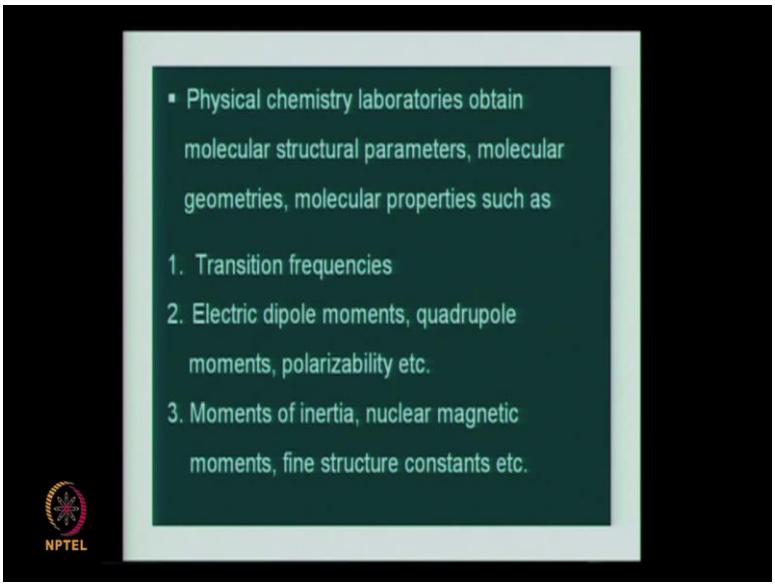

That is as for as the research labs concerned with molecular nature in terms of quantitative detection. Now, also if you think about at the molecular level at a more fundamental level spectroscopic techniques are used to understand the molecular themselves. Why molecules have the shape and the structure and the properties that they have. Molecule having the dipole moment, the molecule having polarizability what do we mean by that and how do we understand them, how do we interpret these properties from our understanding of molecules interaction with radiation. So, if you consider that physical chemistry laboratories use spectroscopic technique particularly, higher solutions spectroscopic techniques, to obtain information on molecular structural parameters, molecular geometric and properties such as transition frequencies we will see them one by one.

We will have to understand what a spectrum means before we can say these are all reasons why we want to study, but the question is there is a motivation for understanding the subjects. So, these are some of the reasons with which we should study this particular subject. Electric dipole moments of molecule; there are properties called quadruple moments molecules, polarizabilities the extent which a molecule can be shaped or de shaped by the presence of an external electric field can be structural changes, can be introduced electrons can be influenced, all these things are contained in the property called polarizability. The molecular moments of inertia very similar to the moments of inertia with it objects, the moments of inertia give us information on the molecular

structure and the angles between various bonds, chemical bonds with the geometrical nature of the molecular. The magnetic moments one of the most important branches of spectroscopy is the nuclear magnetic resonance spectroscopy which, if you are not familiar. You are familiar in a certain way that when you go to the doctor and sometimes when you are prescribed to get a MRI scan the magnetic resonance imaging scan the instrument works with the fundamental principles which you will understand here in the form of magnetic resonance spectroscopy. Some of you have been to the lab though it is as fairly costly experiment to perform to find out what happens in your body. But MRI for example, it is a famous example for you, X ray is another famous example for you that spectroscopic techniques are used on day to day basis

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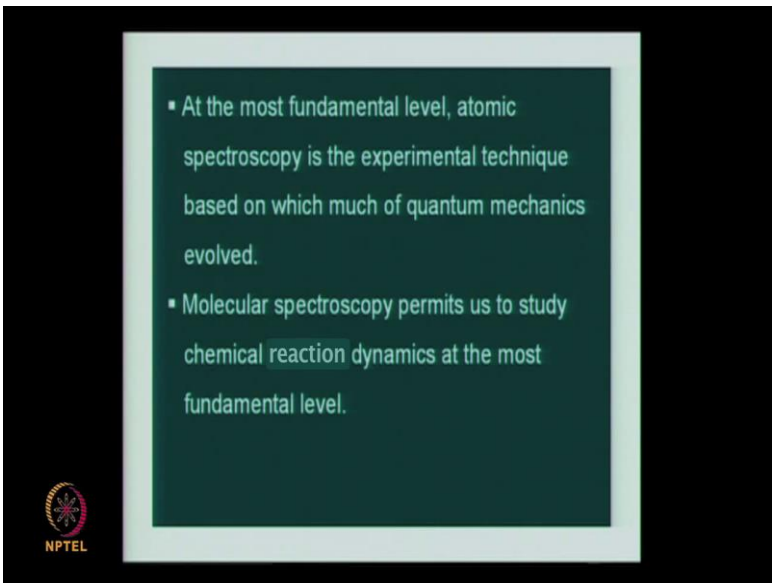

At the most elementary level that is of the microscopic level, if we really want to understand, why a chemical reaction takes place then it is very important to see how a chemical reaction evolves. The spectroscopy that we study and the advanced techniques based on the various methods allow us to map how a molecule under goes changes during a chemical reaction. These days it is possible to photographically map the changes that take place using laser pulses a branch known as the Femtosecond spectroscopy. It is a very, very advanced technique and it is one of the most fundamental techniques to explain what happens in a chemical reaction can we identify intermediate and so, on.

So, at the microscopy level there is; obviously, the reason because all quantum mechanical considerations all results that you derived from the quantum mechanics can be verified by this experimentally techniques. Therefore, the molecules spectroscopy permits us to study the reaction dynamics at the most fundamental level .