Chemistry I
Introduction to Quantum Chemistry and Molecular Spectroscopy
Lecture 3
Electromagnetic Radiation: Oscillating Waves of Electric and Magnetic Fields

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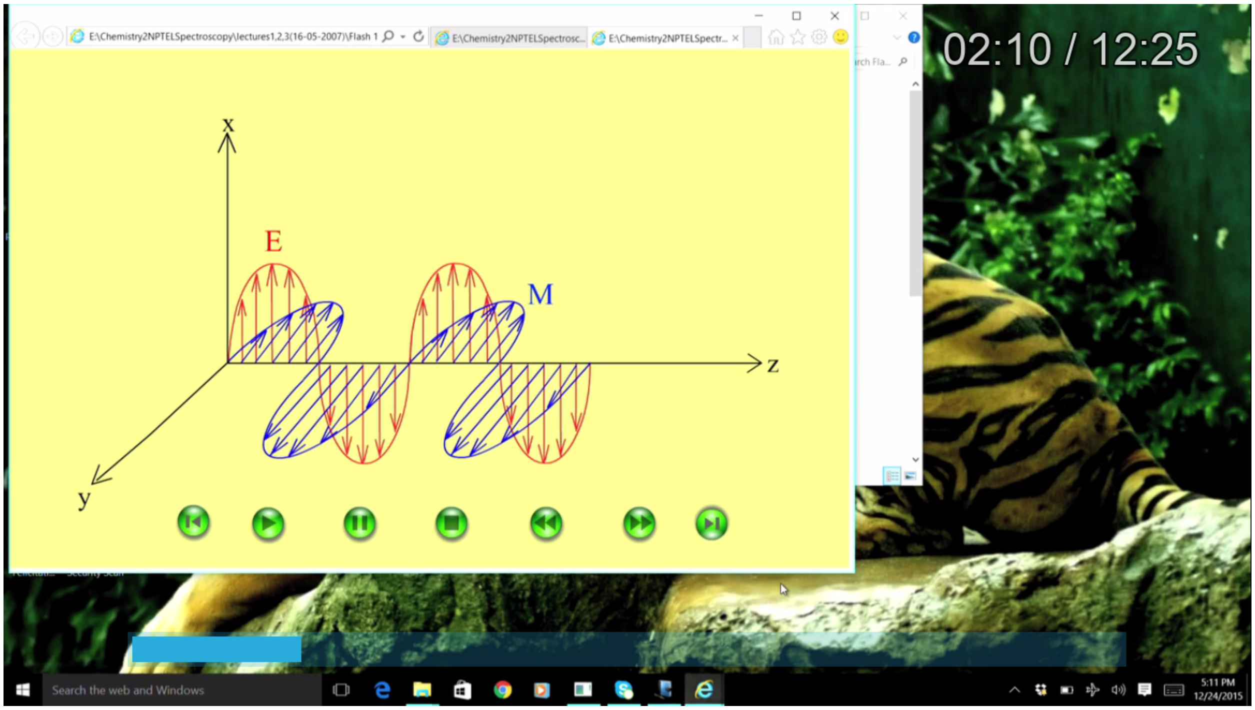
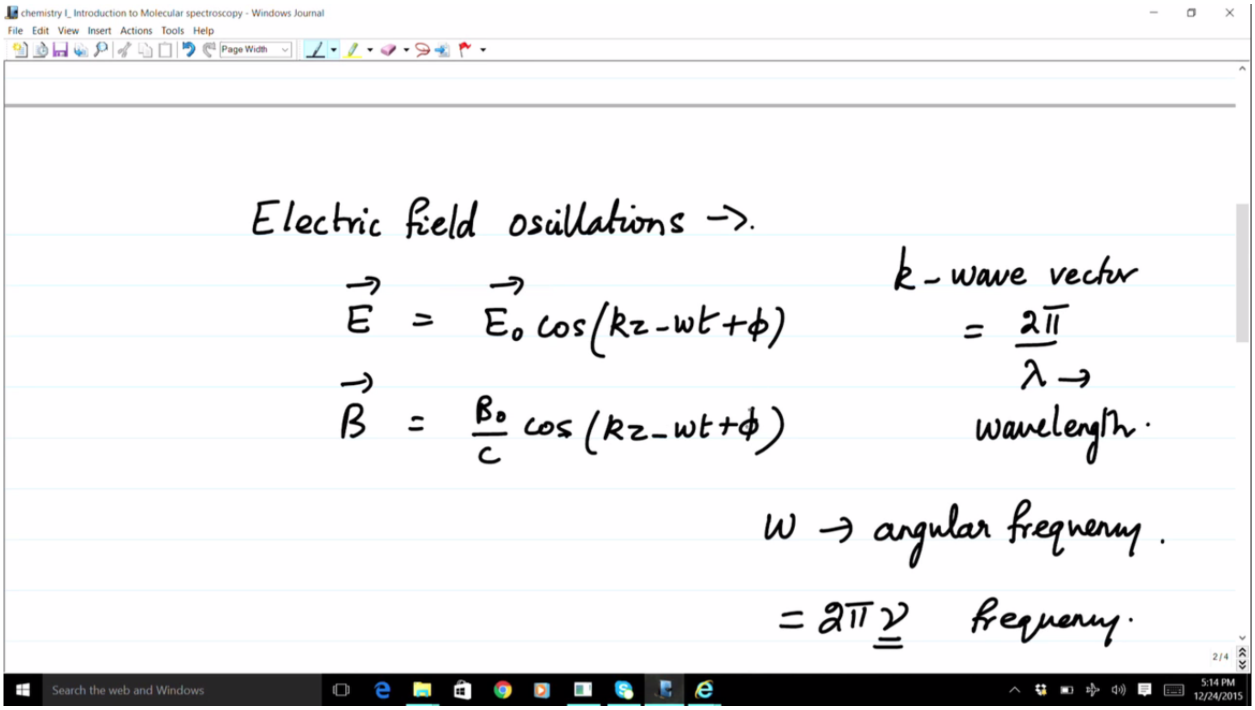
Welcome to the lectures on molecular spectroscopy. In this week which is the first week we have a few introductory concepts and the lecture is on the basic properties that we should know of the electromagnetic radiation. Now spectroscopy is the interaction of electromagnetic radiation with matter of four properties of electromagnetic radiation such as the electric field, the magnetic field, their variation in time and how the wavelengths and the frequencies of these radiation are connected to the energies and so on is the focus of this lecture.

So let me first introduce you to the oscillating electric and magnetic fields as waves. So what you see here is an axis system XYZ rectilinear in which the time-dependent oscillations of the electric and magnetic fields are shown as waves in mutually perpendicular directions you can see that the blue oscillation is marked as the magnetic field and it's in the YZ plane. The red oscillations are marked as the electric field and that's in a plane perpendicular to the YZ namely the XZ axis, XZ plane and both of these waves the oscillations both of these oscillations, the red and the blue oscillations are perpendicular to the direction of propagation which is the propagation marked as the Z direction. So electric field and magnetic fields of an electromagnetic radiation oscillate in time with the same frequency.

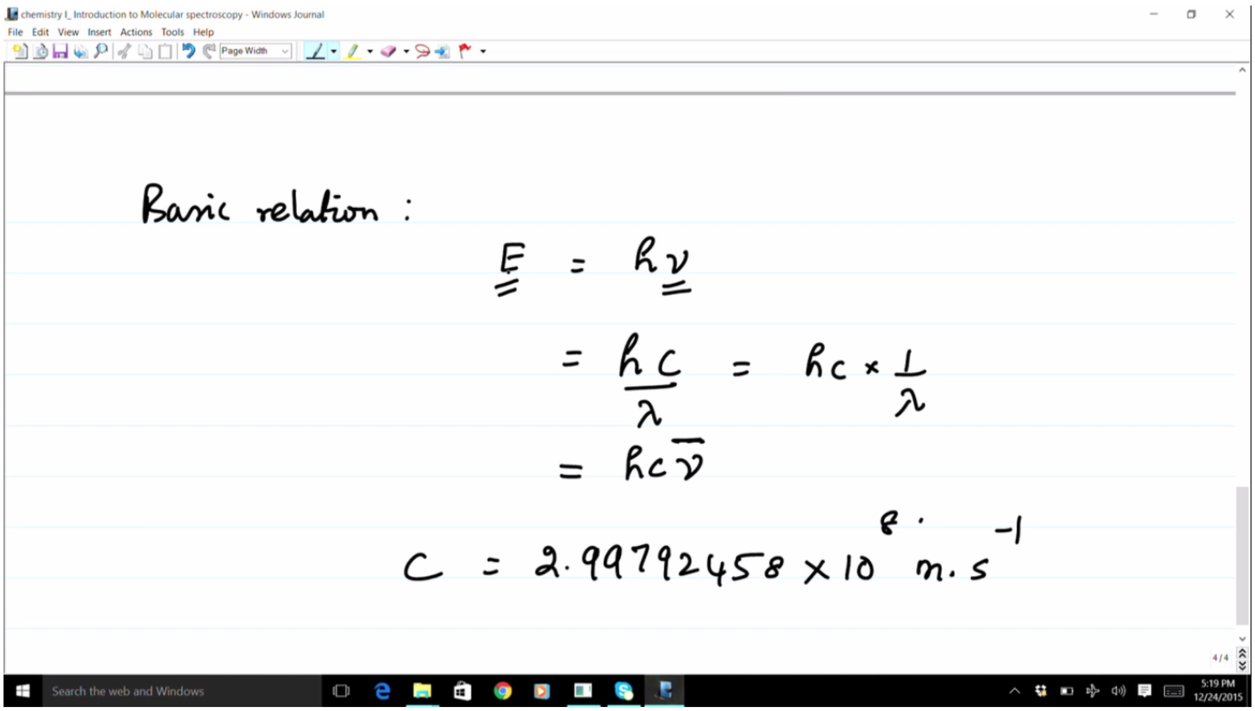


So this is the purpose of showing this animation and you can see that when you want to play this again you can see how the waves are shown as oscillating in time. This is a classical picture. Albert Einstein of course came up with the theory that light is, it consists of what are called the packets and the packets have specific energy which are proportional to the frequency of the oscillation. So let's now introduce some of those terms. The oscillation of the electric field in time and in space is typically given by a simple harmonic oscillation namely the electric field which is a vector is given in terms of the magnitude or the amplitude of the wave E0 and a cosine k where k is called the wave vector for the wave and it's given by the wavelength of the wave we will see that in a minute. Lambda is the wavelength. So E is E0 of cosine kz minus Omega t and Omega is known as the angular frequency of the wave. It has to be because k has to have the inverse dimension of z which is length and Omega has to have the inverse dimension of t and you can see that the Omega angular frequency is given by this formula 2 pi times nu where nu is the frequency of oscillation. The magnetic field B is given in a similar fashion with an amplitude B0 by c and a cosine oscillation also given by kz minus Omega t. In both cases I have put in a factor called Phi which is usually a phase shift or a phase difference for the waves. Shift that's a starting point of the wave we can determine.



Now there are two or three properties that I have introduced the wave length, angular frequency, and I will also introduce a unit called wave number. Let's see that. The frequency of the wave nu is basically the number of waves that pass a point in a given in a unit time. Let's just see that in the oscillation here. You can see that the frequency is the number of waves for example passing to this point the blue dot that you see here in a unit time. So it's number per unit time. The number of full waves that pass a given point in one second. Here the time is in seconds and the number per second is called the frequency. The other definition that you have to keep in mind is the wavelength. Wavelength is denoted by the symbol lambda and being in length it has the unit of length and usually in terms of meters or subunits of meters like millimeter or micrometer or nanometer and so on but the wavelength is the length of one oscillation. The wave number is the number of such waves in a unit length. So let's see that the wavelength is the length of a wave a full wave and you can see that a full wave obviously is marked by points of repeated occurrence successive occurrence for example between the two crests or between the two troughs or between the starting point of the wave at some time the amplitude being 0 or some amplitude and going through one full cycle whatever is the distance that length is called the wavelength. So this is the lambda is the same whether it is between these points or whether it is between these points or is between these points. So it's successive occurrence therefore it's the length of one full wave. What about wave number?

Suppose we have a unit length marked by a distance here. Let's see if this is a unit length then in that length to the number of waves. So you can see immediately that the wavelength and the wave number are inverses of each other because one is the length of the wave the other is how many such waves are there in unit length. So these are elementary ideas but nevertheless these are important. So we have three units namely the frequency. Three quantities namely the frequency, the wavelength and the wave number which is usually written as a nu bar and wavelength is that with the dimension numbers per unit length or with the unit meter inverse and these are connected to each other through the speed of light in vacuum which of course has a value C, has a value 2.99792458 times 10 to the 8 meters per second okay that's a speed of light in vacuum and the relation between the frequency and the energy of a photon which in Einstein's formulation the electromagnetic wave is treated as a collection of packets and the energy of individual packet or the photon is given by the frequency and h is of course the Planck's constant. And frequency and the wavelength are related to each other by the speed of light C is equal to nu lambda and if you substitute for that you see that energy is hc by lambda or it's hc times 1 by lambda therefore you can see that the energy is proportional to the wave number the energy is proportional to the frequency but the energy is inversely proportional to the wavelength. So these are fundamental relations in treating the electromagnetic radiation as a wave.



For the course on spectroscopy we shall use electromagnetic radiation with the classical property that we are familiar with that it is a wave. The reason being that such an approximate formulation is sufficient to understand at a fairly detailed level what happens to the transitions and what happens to the intensities of the spectral lines and so on of course an exact or a more accurate even description of the electromagnetic radiation if it is done in the form of photons will require creation of photons and annihilation of photons and so on and that's taking us more into quantum mechanics. Therefore the spectroscopy that we will do is a combination of two ideas namely the energy levels of the molecules being treated quantum mechanically and the electromagnetic radiation treated as a classical entity. So it is a semi-classical model that we will have.

Spectroscopy, our approach to spectroscopy is that of a semi classical models. Semi classical obviously implies that it's both classical and also not classical. What is not classical we treat the molecules as a quantum mechanical system and therefore we study the molecular energy levels by solving the quantum mechanical equation namely the Schrodinger equation and therefore molecular energy levels are treated using quantum mechanics. The semi-classical part the classical part of the semi-classical is that of the treatment of electromagnetic radiation as consisting of waves of oscillating electric field and oscillating magnetic field and not necessarily as photons and then invoking the quantum electro dynamical theory of the electromagnetic radiation. We don't do that that's what much more advanced work and for the current spectroscopic model and for this and probably a couple of other courses in chemistry the semi classical model is sufficiently accurate. Therefore, please remember molecules by quantum mechanics radiation by classical mechanics.