Atomic and Molecular Physics
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Lecture - 46
Vibration of a molecule

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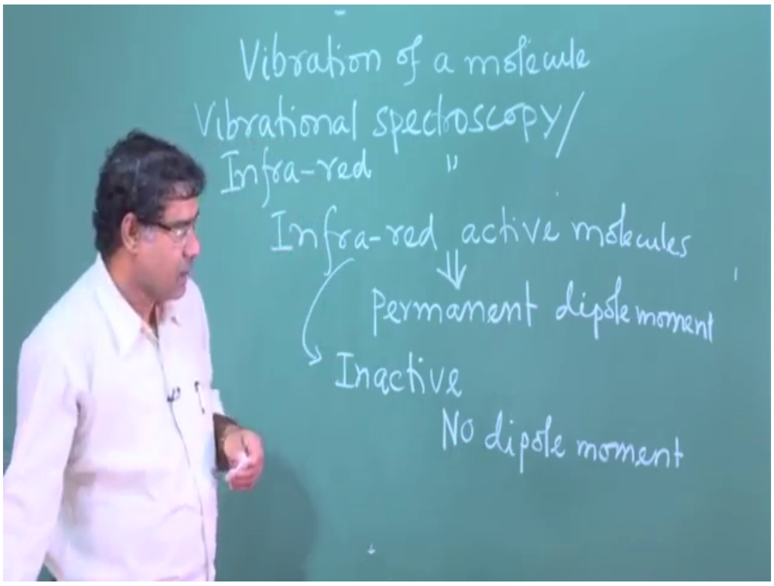

So, today we will learn about Vibration of a molecule, vibration of the molecule. We have seen the rotation of the molecule and corresponding energy levels and spectral lines. So, vibration of a molecule in this case also in this case also this the molecule has to have permanent dipole moment, then it will be infrared active.

So, it is similar to rotational of a rotation of the molecule, rotational spectroscopy as well as it is called microwave spectroscopy. So, in case of vibration of a molecule, so, we get basically vibrational spectroscopy or it is called infrared spectroscopy.

So, some molecules are infrared active and some are infrared inactive, infrared active molecule, active molecule.. So, which are having the permanent dipole moment. So, this for this case that molecule should have permanent dipole moment ok. And it will be infrared inactive infrared inactive infrared inactive, when molecule will not have.

So, no dipole moment in this case no dipole moment or better it is it is better it is it is it is to say that the there should be change of dipole moment, fluctuation of dipole moment due to vibration. If so, then it is infrared active molecules. If there is no change of or fluctuation of dipole moment during vibration, then it will not be microwave active molecule ok.

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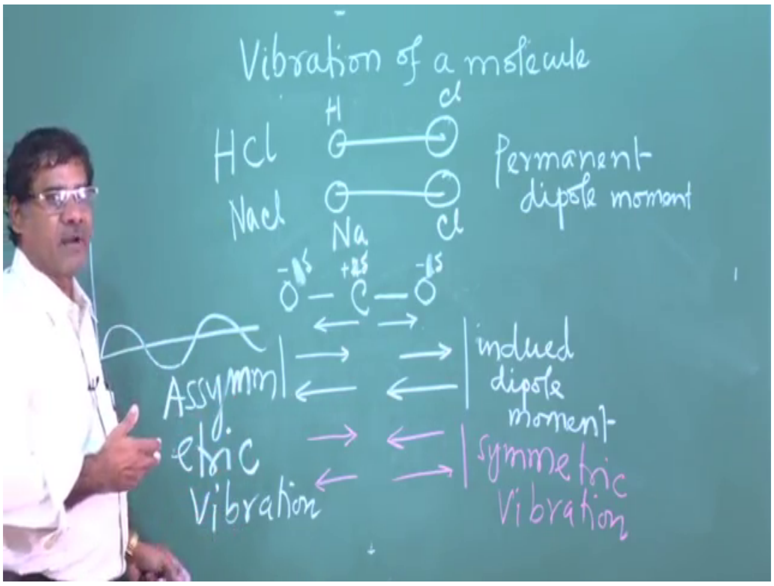

So, we will give example that like this we have we have seen that in case of Hydrogen Chloride. So, this two heterogeneous nucleus basically heterogeneous nucleus having the permanent dipole moment, so this sodium hydrogen and chlorine; so, it has permanent dipole moment. So, it is infrared active, similarly sodium chloride sodium chloride ok. So, it has permanent dipole moment. So, basically in this case it has permanent dipole moment ok.

So; obviously, it is microwave active, but sometimes this molecule it do not have permanent dipole moment like say carbon dioxide ok. Say carbon dioxide it has no permanent dipole moment, but due to vibration due to vibration it may happen that there will be induced dipole moment and with vibration or with time this induced dipole moment induced dipole moment fluctuates and then that molecule will be micro infrared active.

So, in case of permanent dipole moment there is no question that all the time it is micro active infrared active right, in case of in case of in case of infrared active. So, this molecule as if so, in this configuration it has no permanent dipole moment ok. So, that you know why it is have it has no permanent dipole moment. So, here is a minus 2 delta charge, here is minus 2 delta charge ok, here plus 4 delta charge ok. So, or I can or if you if you think like this minus delta and this minus delta then one can write this ok, so, that the charge balance.

So, now dipole moment here, so, direction is positive to negative direction. So, direction is in this direction and here positive negatives in this direction. So, this equal dipole equal magnitude, but having the opposite direction. So, net dipole moment for this carbon dioxide is 0 ok.

But if it vibrates if vibration is symmetric if vibration is symmetric means this oxygen they are vibrating ok, keeping this carbon at the middle ok. If vibration is symmetric means this oxygen is when it is going this side. So, this oxygen is also going the same direction ok yes. So, what is happening? It is going this direction; it is going this other direction.

So, in this case or just opposite way. So, what is happening? In this case dipole moment, so, it is going this side. So, length is increased. So, the dipole moment will increase ok. And in this case this distance length is decreasing it is going this side. So, each dipole moment will be smaller, this side dipole moment is smaller, this side dipole moment higher.

So, there will be. So, direction is of course, in opposite direction, but now magnitudes are different ok. So, it will show net dipole moment, due to this basically this oscillation this vibration ok. So, if it vibrates like this that it is it is going this side, it is going to this side ok. So, same things so, this will increase. So, dipole moment is higher, this will decrease dipole moment is lower. So, net dipole moment in this direction ok. So, due to this either vibrating in same direction ok either this way or that way. So, in this case there will be induced, there will be induced dipole moment which will change with time.

So, that means, there will be fluctuation of dipole moment with time as I have shown in case of rotation ok in same way. So, this fluctuation with time actually if you plot so, this fluctuation is this will be like this. So, it will interact with the infrared and that is why it will be infrared active molecule ok.

So, if this vibration is different way say. So, it was in same direction, now if it is in opposite direction. So, when it is going this side, other one is this side or other way when it is going this side, other is going other side. So, it is basically now it is going this side and this oxygen is coming this side, so basically compressed.

So, if so, this basically now they are coming towards carbon. So, dipole moment magnitude will be will be different for each one ok. So, total dipole moment will be then there will not be total dipole moment will be 0, there will not be any net dipole moment ok. So, other way when it is stretched expanded vibrating this way going this other side. So, these also increase dipole moment increase, these also dipole moment increase and dipole moment are in opposite direction they are same. So, then it will not be again there will not be any net dipole moment.

So, these call basically symmetric vibration ok. This is called symmetric vibration, symmetric vibration of the molecule and in case of symmetric vibration of the molecule, there will not be any induced dipole moment or there will not be any fluctuation of dipole moment with time.

So, this molecule in that case it will be micro inactive molecule. And in this case this is called basically symmetric asymmetric vibration. This is basically asymmetric vibration; asymmetric vibration ok. So, in case of asymmetric vibration there will be change of dipole moment fluctuation of dipole moment with time. So, then it will be infrared active molecule ok.

So, it depends whether it will be infrared active or it is not infrared active, in case of in case of no permanent dipole moment. So, for those molecules which are not having permanent dipole moment for that molecules also sometimes it is micro infrared active, it may become infrared active when they will have asymmetric vibration.

If they have symmetric vibration, then it will not be infrared active molecule ok. So, from infrared spectroscopy or vibration spectroscopy, one can tell about the vibration of the molecules, whether this molecule is vibrating symmetrically or it is vibrating asymmetrically ok. So, also this vibration may not be only this in along the straight line, it may be this dipole moment change or induced dipole moment or fluctuation of dipole moment ok, it may happen due to bending of the molecule also ok.

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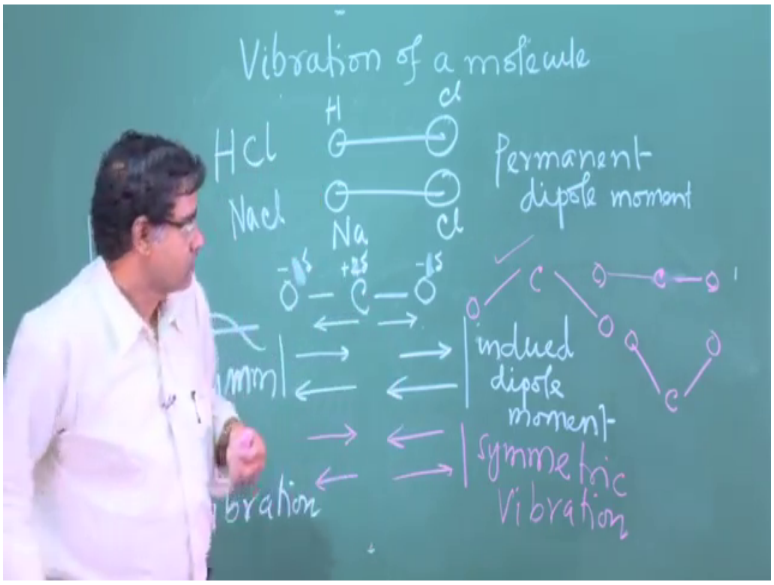

So, in this case if it vibrates oscillates like this. So, if starting is this then ok, then again come straight again come straight ok and next step it is if it is ok. So, if this way also it bends ok. So, this carbon atom carbon atom now 2 oxygen ok, now if it bend going straight, again bend ok.

If due to the bending of the molecule of the molecule with time this also will give the induced dipole moment and there will be fluctuation of dipole moment with time, then also it will be microwave or in case of vibration it is a infrared active molecule ok.

So, due to vibration or due to oscillation in terms of bending or in terms of a symmetric stretching and compression ok, there will be induced dipole moment and due to this induce dipole moment or due to the fluctuation of dipole moment, fluctuation of induced dipole moment with time, the molecules which are not having permanent dipole moment they are also microwave sorry infrared active molecule ok.

So, that generally in case of in case of rotation, it is only the molecules which are having permanent dipole moment; only those molecules are micro active. But in case of vibration of a molecule although there is the some molecules do not have permanent dipole moment, but due to the asymmetric vibration or this bending of the molecules, so, this induced dipole moment fluctuate with time and it become infrared active molecule ok.

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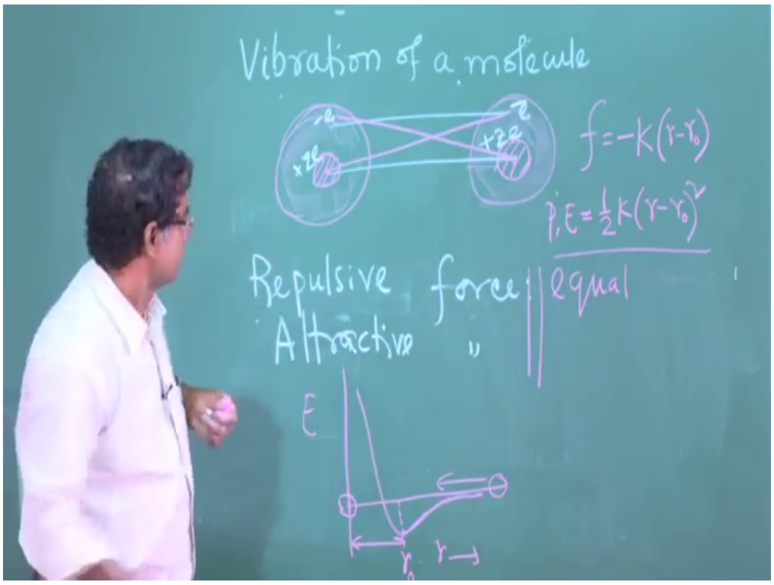

So, now, vibration of a molecule, vibration of a molecule, so, basically one has to understand that this one atom is here. Now if you bring another atom, if you bring another atom towards this atom. So, they form molecule keeping them these 2 molecule 2 atoms in equilibrium distance and that distance is called bond length ok. So, what will be the equilibrium distance that depends on the force?

Two type force will act here, one is say this is nucleus and here distribution of electrons, in this molecule also this a nucleus and this distribution of electron ok. Now when they will come closer then there will be electrostatic force between these two atom.

So, two type of force will act; one is attractive force. So, source of attractive force will be this electron-electron, electron-electron interaction and nucleus-nucleus interaction. So, this source of attractive force sorry, so this it is just opposite. So, let me write this repulsive force repulsive force repulsive force source of repulsive force electron-electron interaction and nucleus-nucleus interaction ok. So, these are positive charge ze plus ze plus ze and these are negative charge electron, electron. So, there will be repulsive force ok.

And, then attractive force there will be also attractive force; attractive force source of attractive force is basically electron-electron nucleus and also this for this atom this nucleus to this electron of the other atom ok, so, nucleus to electron that interaction basically it will be attractive force. Now when you are bring them closure, so, these force will balance, these two force will be equal at a particular distance at a particular distance, then that is it at that distance basically we tells us total energy of this molecule will be minimum total energy of the molecule will be minimum.

So, generally this energy this curve is like this. It is it is really varies like this ok. So, if here this one molecule and another molecule here you are another molecule you are bringing towards this. So, this the r ok; this is the r and this is the energy ok. So, this energy changes like this. So, when you are bringing so, energy is this; it is it is very small ok, then it is changes like this. So, energy become minimum and further if you, so, these distance if I tell this distance is r 0 r 0.

So, when distance is greater than r 0, the energy is higher. If less than r 0 energy is higher ok, but in this side if we see that the change of energy is very sensitive to the change of the distance, so; that means, these two molecules from equilibrium position ok, if you try to bring more closer.

So, the change of energy is very high; rate of change of energy is very high. On the other hand, if you go if you go this other side, if you try to take away from the equilibrium distance then it is energy also increases, but rate of change of increment is slow ok.

So, this force is basically or this energy changes basically is not symmetric, it is asymmetric ok. So, these the these the r 0 is the equilibrium distance. Now from equilibrium distance if you try to if you try to change, if you try to change the distance then it is energy will change, it is energy will change it is yes.

So, it is, so, it will happen during vibration. So, vibration of a molecule basically for a diatomic molecule, molecule is in a equilibrium position, they have bond length, equilibrium distance is r 0, now when they will vibrate when they will vibrate or symmetrically or asymmetrically symmetrically or asymmetrically ok.

So, then there that energy will change and that energy basically potential energy ok and this potential energy if you compare with spring mass system, if you compare with the spring mass system. So, this force, force basically you can write f equal to like spring mass system minus k r minus r 0 ok. And corresponding potential energy potential energy is half k r minus r 0 ok.

So, that will be the energy change potentially change due to the vibration. So, we have a system we have a system when it will vibrate, it is energy will change mainly potential energy we will change and that is this ok.

So, now, we are interested to find out the steps of the molecule which is vibrating; that means, the energy levels with which energy this molecule can vibrate, whether it can vibrate with n energy or the energy is discrete ok, is quantized. So, that is what we would like to find out and that is similar to the rotation case, you have to use the Schrodinger equation and solve the problem and find out the solution.

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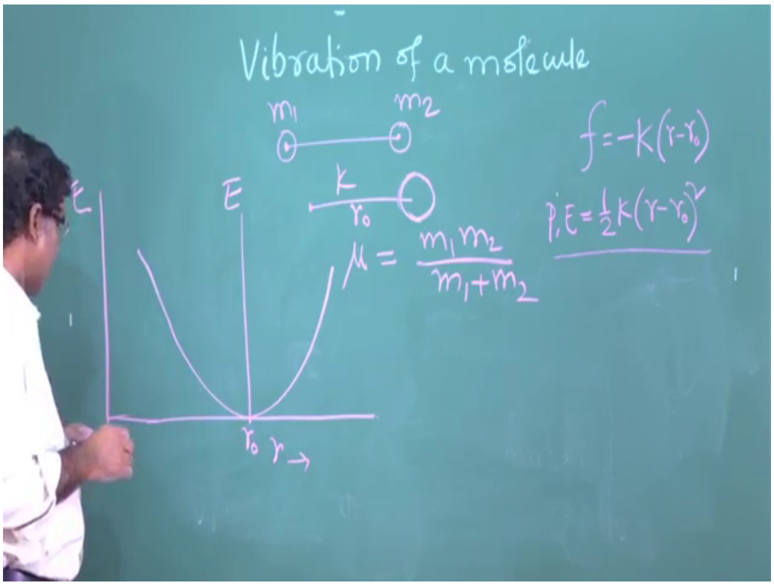

So, now, this vibration, vibration of this diatomic molecule ok, say it is a mass m 1 and mass m 2 ok. So, one can reduce to one can reduce to a, so, two body problem reduce to one body problem right. So, that is already you know.

So, this will be the reduced mass of the system and it will oscillate, it will vibrate like spring mass system ok. So, it is equilibrium distance is r 0, it is reduced mass will be m 1 m 2 m 1 plus m 2 ok. So, now, it is not just simple harmonic motion ok. It is the case of simple harmonic motion despite the spring mass system ok, one body problem ok. So, spring there is a spring constant k ok. So, it is oscillating.

So, this will be the potential energy and this potential energy, if you plot if you plot this potential energy if you plot, it will be it will be like this equal plot. So, these the energy, these the energy and these the distance r ok.

So, these are energy. So, this position is r 0 ok. So, when the at the r equal to r 0 this energy is minimum, when r is changing it is energy is higher, but these are symmetric ok. So, this is the harmonic oscillator potential or if the potential energy changes like this ok, so, this then we tell that is the simple harmonic motion, simple harmonic motion or simple harmonic oscillator, it is a simple harmonic oscillator.

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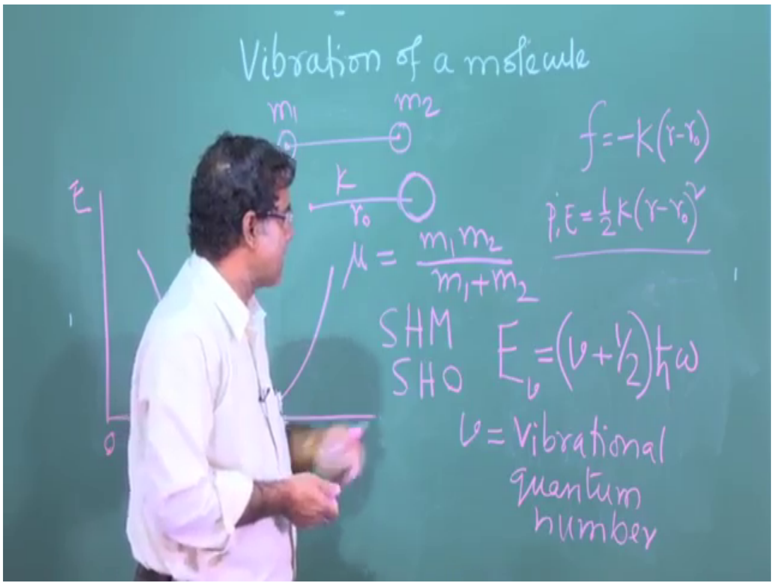

So, vibration of a molecule so, one can converted the this problem to a simple harmonic oscillator it is a it is behaviour is just like a simple harmonic oscillator and to solve simple harmonic oscillator the standard problem in quantum mechanics and solution is known to you hopefully.

So, this it is energy expression if you solve using this potential energy to solve the Schrodinger equation for simple harmonic oscillation. So, this you will get energy E v equal to v plus half v plus half h cross omega ok.

So, this the v is a is a it is called vibrational quantum number vibrational quantum number like in case of rotational quantum number j we have used; here similarly v is vibrational quantum number ok. Vibrational quantum number and the energy of this oscillator or this molecule, which is vibrating this it states or it energy level is quantized and this energy levels will follow this relation ok. So, I will continue the discussion let me stop here.

Thank you.