# Group Theory Methods in Physics
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## Lecture – 28
## Selection Rules and Molecular Vibrations

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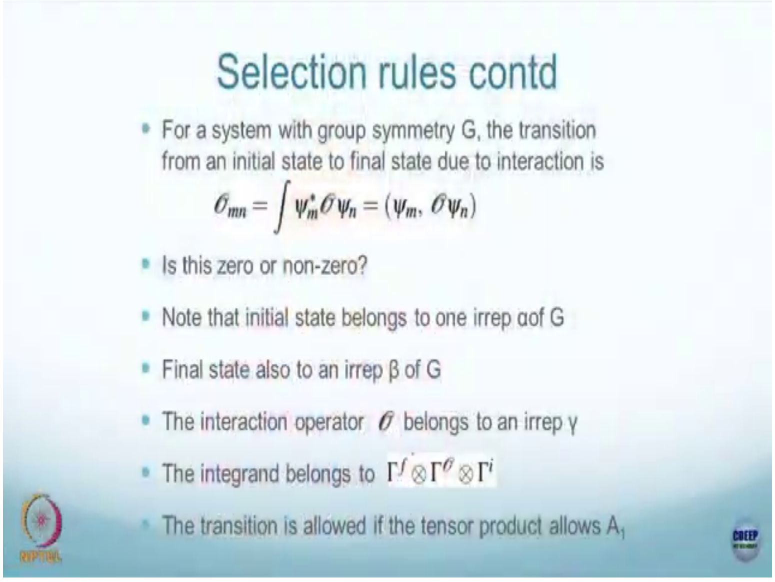

## Selection rules contd

- For a system with group symmetry G, the transition from an initial state to final state due to interaction is
$$\mathcal{O}_{mn} = \int \psi_m^* \mathcal{O} \psi_n = (\psi_m, \mathcal{O}\psi_n)$$
- Is this zero or non-zero?
- Note that initial state belongs to one irrep αof G
- Final state also to an irrep β of G
- The interaction operator $\mathcal{O}$ belongs to an irrep γ
- The integrand belongs to $\Gamma^f \otimes \Gamma^{\mathcal{O}} \otimes \Gamma^i$
- The transition is allowed if the tensor product allows $A_1$

For a system with group symmetry G, I have just said all these things, now I am just repeating for summarizing. The transition from an initial state to due to interaction, interaction is given by some operator O; there is an initial state n and a final state m and I want to find whether this result is going to be zero or nonzero, it is what I said. So, you have to remember that the initial state belongs to one irrep, let us call it as alpha. Final state should belong to another irrep, need not be the same irrep, right.

This transition was not between the same irrep, this transition is between the same irrep. So, it does not really matter, it belongs to one irrep alpha initial state; final state belongs to another irrep beta. Alpha and beta could be same, alpha and beta could be different ok. And then the interaction operator also belongs to one of the irrep; if the interaction of a operator is associated with an observable, so that also you can give it as a irrep. Idea is that, the integrand involves tensor product of the irrep associated with the final state, irrep associated with the initial state, irrep associated with the observable ok.

The transition is allowed if the tensor product allows A 1, clear. In all these 1 D, you just got A 1, right. If you are doing C 4 v, there is a E cross E which could give you A 1 plus A 2 plus something, right. So, you need to see at least A 1 should be there in the tensor product; the irrep one of the irrep should be a A 1, then only it will be nonzero. So, this thing which I have written, in principle could be a linear combination of; if it had a combination this will be zero, but that could give you nonzero.

So, in this 1 D there is no problem, you can see that from this table that it is only A 1; you do not get a linear. Why you do not get a linear combination? 1 D irrep with 1 D irrep has to give you only 1 D irrep, it cannot give you a 2 D irrep to write a linear combination; but E cross E can give you. So, let us do some examples.

Student: Do we have (Refer Slide Time: 3:09).

So, such things happen then we need to figure out how to do it; but right now I am saying most of the operators will have some associated with the symmetry of the system ok. I agree with you ok. C 4 v is the two dimensional particle in a box ok.

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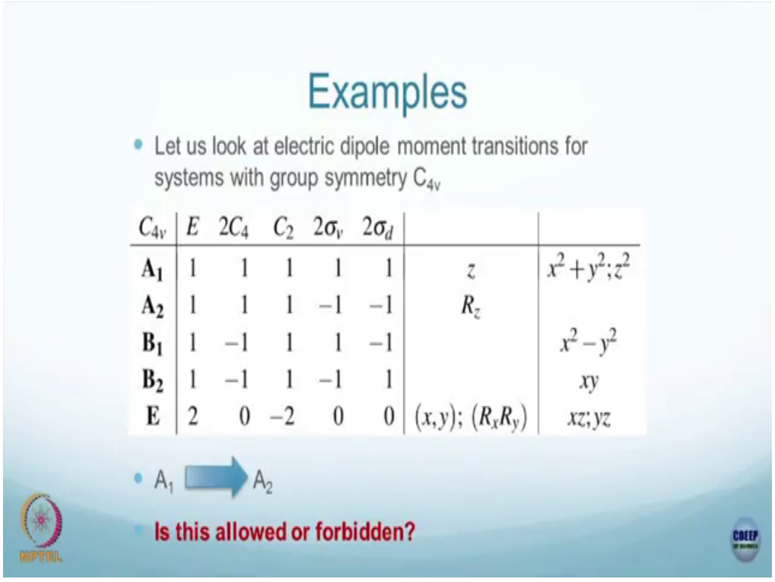

## Examples

- Let us look at electric dipole moment transitions for systems with group symmetry $C_{4v}$

| $C_{4v}$ | $E$ | $2C_4$ | $C_2$ | $2\sigma_v$ | $2\sigma_d$ | | |
|---|---|---|---|---|---|---|---|
| $\mathbf{A_1}$ | 1 | 1 | 1 | 1 | 1 | $z$ | $x^2+y^2; z^2$ |
| $\mathbf{A_2}$ | 1 | 1 | 1 | −1 | −1 | $R_z$ | |
| $\mathbf{B_1}$ | 1 | −1 | 1 | 1 | −1 | | $x^2-y^2$ |
| $\mathbf{B_2}$ | 1 | −1 | 1 | −1 | 1 | | $xy$ |
| $\mathbf{E}$ | 2 | 0 | −2 | 0 | 0 | $(x,y); (R_x,R_y)$ | $xz; yz$ |

- $A_1$ → $A_2$
- **Is this allowed or forbidden?**

So, if you take C 4 v and look at electric dipole moment transition for system with C 4 v group symmetry, you have to first have this character table with the binary basis, primary basis and so on, ok.

So, first of all initial state let say is an A 1 irrep, final status in A 2 irrep and I want this to be triggered by the dipole moment operator. Dipole moment operator belongs to the x and y component belong to E dimensional representation, z component belongs to A 1 representation, right. If you take the z component, you can show that A 1 times A 1 times A 2 is A 2, right you agree ok.

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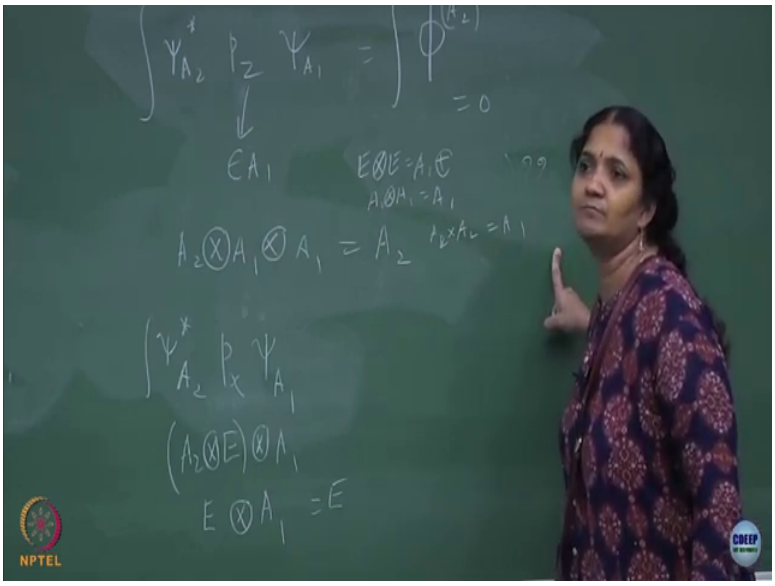

$$\int \Psi^*_{A_2} P_z \Psi_{A_1} = \int \phi^{(A_2)} = 0$$

$$P_z \in A_1$$

$$E \otimes E = A_1 \oplus \ldots$$

$$A_1 \otimes A_1 = A_1$$

$$A_2 \otimes A_1 \otimes A_1 = A_2 \quad A_2 \times A_2 = A_1$$

$$\int \Psi^*_{A_2} P_x \Psi_{A_1}$$

$$(A_2 \otimes E) \otimes A_1$$

$$E \otimes A_1 = E$$

The initial state belongs to an A 1 irrep; if suppose I want to look at the z component, it belongs to also A 1 irrep, ok. So, you can see that A 2 times A 1 times A 1 will be; A 1 and A 1 are like identity, it has to be A 2, right. So, you can write this as sum phi which belongs to A 2. And the great orthogonality theorem says that; A 2 is not A 1, it has to be 0, clear.

Which wave function in the two dimensional particle in a box belongs to A 2? The one with eigenvalue minus 1, which one will happen; n being odd or n being even, you can check it. N being even may be A 1 and n being odd will be A 2 or something just check; check which one is the one which can belong to the and then you can do that elaborately and check that these two answers are actually one and the same, is that clear.

Other thing is P x and P y; P x and P y belong to E, right. So, if I try to take psi star A 2 P x or P y, I do not worry. So, this should be element of A 2 tensor product E tensor product A 1, right. A 2 with E you can check in the character table, A 2 with E is again E ok; you can multiply in the character table. If you multiply A 2 with E; because the negative 1s are all 0 here, A 2 with E is exactly E again.

So, A 2 with E is E and E with A 1 will be again E; you all with me. What does it tell us? This transition whether it is x component or y component will also not happen. So, once I have found all the components is not possible, I make this statement that A 1 to A 2 transition; I am not even saying, I do not even know what are the levels and what are the energy, I am just saying if the initial state belongs to an irrep A 1 and final state belongs to an irrep A 2.

Due to an interaction which is the electro electric dipole moment operator ok, none of the components will trigger such a transition from A 1 irrep to A 2 irrep. So, it is a forbidden process, are you all with me. I do not done any algebra anything, I am just arguing some group theory character table and using great orthogonality theorem that has to be 0, I am just saying this like this is.

This is something which you also do in quantum mechanics, Wigner Eckart theorem in the continuous version is mimicking this ok. So, we will see at that point exactly what is happening there. This in the discrete context using great orthogonality theorem, forces that the integrand has to belong to a unit representation or it should at least contain unit representation ok. If you had e cross e cross e, it could give you a lot of linear combination, it should have A 1 in it; if it has A 1 it is nonzero, if it does not have A 1 it is going to be 0 ok.

So, this is one thing which you have to remember and sometimes what people do is, that they just confined to the initial state and the final state; sorry initial state and the operator or final state and the operator and see what you get out of this. If it is same as the initial state ok, you will you can be sure that you will get a A 1 unit ok. If you have seen E cross E will definitely have an A 1. If you have an A 1 cross A 1, you will definitely have an A 1; A 1 cross A 2 sorry A 2 cross A 2, it will definitely have an A 1.

So, the same irrep tensor products typically will contain A 1. So, this has some other combinations, but any same representation tensor product will contain an A 1 ok. So, you could do a combinations of these, not to do all the three, two of them tensor product; if it is same as this one, here anyway it is A 1. So, it is trivial, but suppose this was A 2; then you know this product if it is A 2 or if it contains A 2, you can still argue that you will have the transition allowed, ok.

This is alternate way of doing, just looking at tensor product of one initial state with the operator; if you get in that irrep, the same as the final state irrep then you get this argument that this will be associative properties all I am saying, ok.

Student: Maam.

Yeah.

Student: (Refer Slide Time: 11:23) instead of if that last A 1, if greater than (Refer Slide Time: 11:27).

Yes.

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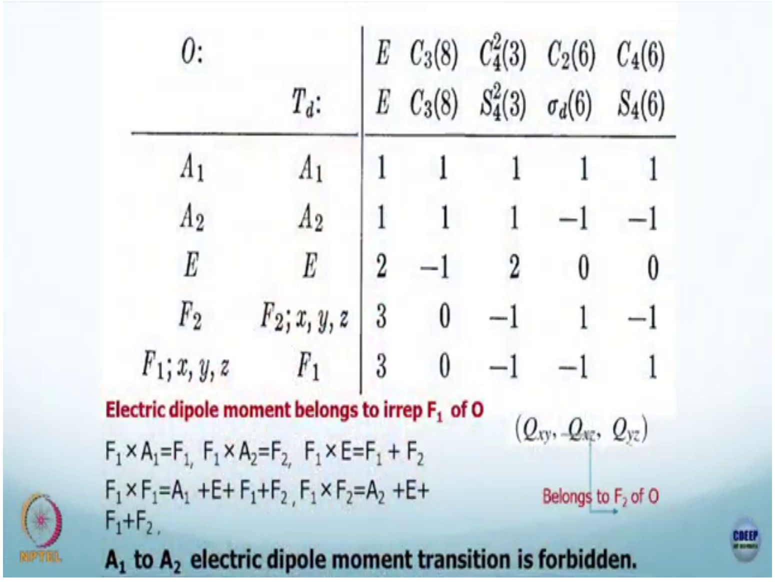

| O: | $T_d$: | $E$ | $C_3(8)$ | $C_4^2(3)$ | $C_2(6)$ | $C_4(6)$ |
|---|---|---|---|---|---|---|
| | | $E$ | $C_3(8)$ | $S_4^2(3)$ | $\sigma_d(6)$ | $S_4(6)$ |
| $A_1$ | $A_1$ | 1 | 1 | 1 | 1 | 1 |
| $A_2$ | $A_2$ | 1 | 1 | 1 | −1 | −1 |
| $E$ | $E$ | 2 | −1 | 2 | 0 | 0 |
| $F_2$ | $F_2; x, y, z$ | 3 | 0 | −1 | 1 | −1 |
| $F_1; x, y, z$ | $F_1$ | 3 | 0 | −1 | −1 | 1 |

Electric dipole moment belongs to irrep $F_1$ of O

$(Q_{xy}, -Q_{xz}, Q_{yz})$

Belongs to $F_2$ of O

$F_1 \times A_1 = F_1$, $F_1 \times A_2 = F_2$, $F_1 \times E = F_1 + F_2$

$F_1 \times F_1 = A_1 + E + F_1 + F_2$, $F_1 \times F_2 = A_2 + E + F_1 + F_2$.

**$A_1$ to $A_2$ electric dipole moment transition is forbidden.**

Student: (Refer Slide Time: 11:29) some of A 1 and A 2 will give nonzero.

If it contains A 1 in that sum, you still get it to be nonzero.

Student: To be.

Get it to be nonzero. So, as an example I put one more complex example here. So, let us look at the octahedral group, which is some of you have tried to work out this character table. You know that as a group symmetry there is some isomorphism between octahedral group and the tetrahedral group with this diagonal mirrors right; 24 elements, both of them have 24 elements.

Octahedral group is a pure rotation group; this T d group has improper reflections also ok, there is some subtle difference. So, that is why I have put the first line as octahedral group elements, which is pure rotations and then the second line as the tetrahedral group elements which involves roto reflection in it, ok. Character table are one and the same, ok. And we can now look at where is the x y z component fitting in, it turns out that the x y z component fits into the irrep F 1 for the octahedral group, ok.

You can start doing F 1 times A 1 see what happens; I said no with unit representation F 1 times A 1 is F 1, F 1 times A 2 will turn out to be F 2 and so on. So, you can start doing this exercise; leave it you to check this ok. In the character table you know how to do the, the left hand side will be reducible F 1 cross E will be 6 cross 3 into 2 6 cross 6 matrix and it will be a direct sum of 2 3 cross 3 irreps. These things you can work it out by looking at this character table.

Once you have this all these things, the tensor product of three things which we want to do becomes easy. If you have it on your screen, all possible tensor products from looking at this character table; then you can start arguing which transition is allowed which transition is forbidden, ok.

According to this diagram and the basis which have written; I have just written the primary basis, F 1 has electric dipole moment operator. So, if you want to look at this transition between A 1 and A 2 due to F 1; F 1 times A 1 is F 1, it is not equal to A 2. So, you will never be able to achieve A 2 out of it. So, it will be forbidden, is that clear.

Similarly you can also use the Q x y, Q x z and Q y z as the three dimensional irrep which belongs to F 2 of the octahedral group and you can show that, you can start looking at whether there is a transition due to elect quadrupole moment itself, ok. I will give you some problems to work on these that way you get a feel of how to do things, some one or two problems on selection rules and that will clarify how the selection rule works, is a theme clear.

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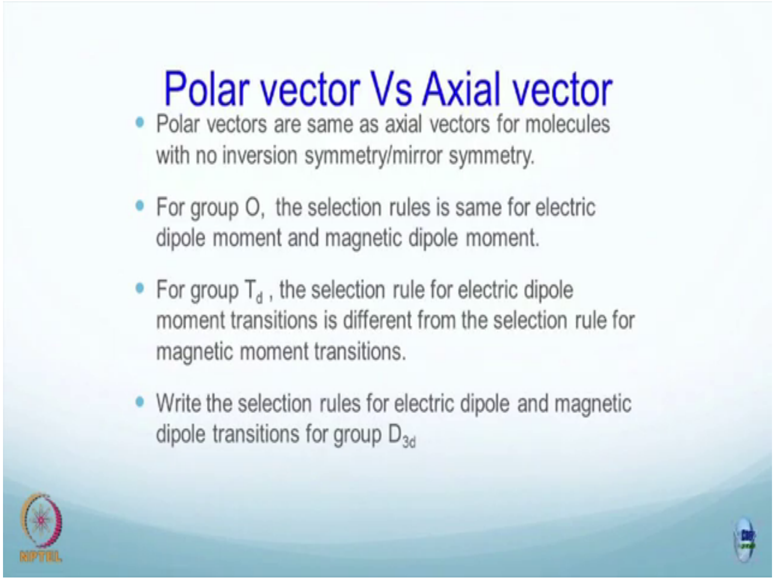

## Polar vector Vs Axial vector

- Polar vectors are same as axial vectors for molecules with no inversion symmetry/mirror symmetry.
- For group O, the selection rules is same for electric dipole moment and magnetic dipole moment.
- For group $T_d$, the selection rule for electric dipole moment transitions is different from the selection rule for magnetic moment transitions.
- Write the selection rules for electric dipole and magnetic dipole transitions for group $D_{3d}$

So, this subtlety I have already said, whenever you have only pure rotation you cannot distinguish a polar vector from axial vector. But once you have improper transformation like reflections, then axial vector is going to be different from polar vector. And this I will give it as an assignment for you to do D 3d, how to find the selection rule for electric dipole and magnetic dipole transition. So, you take the character table with the basis from the literature and then you work it out, ok.

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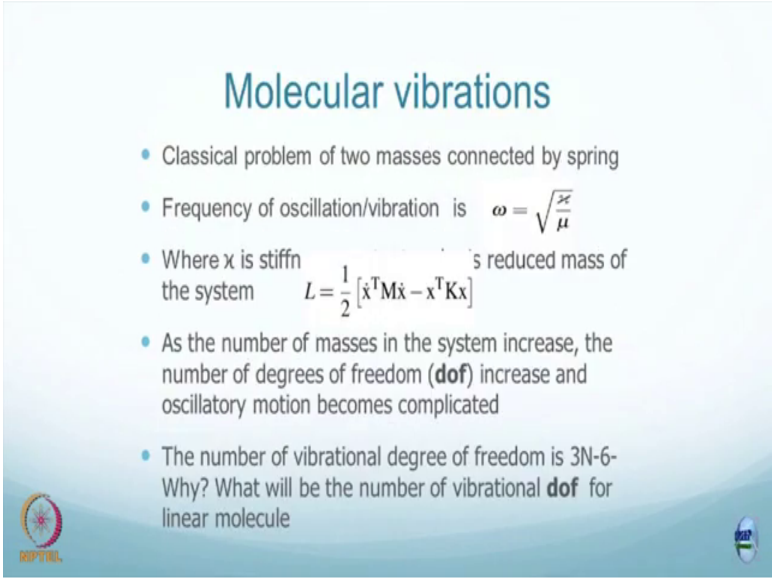

## Molecular vibrations

- Classical problem of two masses connected by spring
- Frequency of oscillation/vibration is $\omega = \sqrt{\frac{\varkappa}{\mu}}$
- Where ϰ is stiffn s reduced mass of the system $L = \frac{1}{2}[\dot{x}^T M\dot{x} - x^T Kx]$
- As the number of masses in the system increase, the number of degrees of freedom (**dof**) increase and oscillatory motion becomes complicated
- The number of vibrational degree of freedom is 3N-6- Why? What will be the number of vibrational **dof** for linear molecule

So, then the next other application of what we did for character table basis states and so on, is to look at vibrations in a molecule, ok. A molecule is made of atoms, you can treat that the atoms are connected by kind of a spring with stiffness. They are all going to undergo various vibrations. I am not looking at translation, I am not looking at rotations; I am only looking at relative vibrations.

Suppose you had two atoms together, it can either go; you know there is only one direction in which it is going to oscillate and you get this characteristic frequency, right which is something which you all do. If you had a two atom, you can go into a reduced mass system and treat as if it is undergoing a simple harmonic motion with frequency omega.

Student: There will be two omega, right (Refer Slide Time: 17:32).

Which one?

Student: Two, there will be 2 omega right one translation (Refer Slide Time: 17:36).

No the translation I am not looking at, translation is both going together; the vibration is what I am looking at, both coming in and going out, is that clear. This going is a translation, I am not looking at it, good; some things are getting erased here, so it is ok. So, what I am saying is that there is a classical problem of two masses connected by a string, by a spring actually of stiffness kappa.

And you know that there is a definite well known frequency for two masses and that is given by the stiffness constant and the reduced mass, you know this; vibration slight displacement where it creates vibration, not the translation mode as he was saying. But suppose you start increasing the number of masses in the system and need not be linear, it could also be non-linear like molecules, like ammonia molecule or water molecule; then they also have vibrational degrees of freedom, besides translation and rotation which I am going to remove.

How do I find those vibrational degrees of freedom? I will not be able to find the frequencies, but I should be able to find how those atoms are going to vibrate which belongs to different vibrational modes. So, as the number of masses increase, the oscillatory motion; if you give a slight disturbance to the molecule it undergoes oscillatory motion. It will be very complicated, I will show you a video; just it is there on the net, but it is nice to see in this context of what you do as an algebra. So, the oscillatory motion is very complicated beyond two masses, you know you have to start working it out.

I am sure you would have done tri linear molecule in your class, in classical mechanics. And number of vibrational degrees of freedom, if there are N atoms; 3 N will be the total degree of freedom in three dimension. Three overall translation you can remove, all the atoms translated by a constant vector is not a degree of freedom and there are three directions for translation. Similarly there are three directions for rotations, you can rotate you remove them, ok.

So, the number of vibrational degrees of freedom for such a molecule with these atoms is going to be always 3 N minus 6. If it is a linear molecule, one of the rotation about that axis is not there; so you do not have three rotational degrees of freedom, only 2 rotational degrees of freedom.

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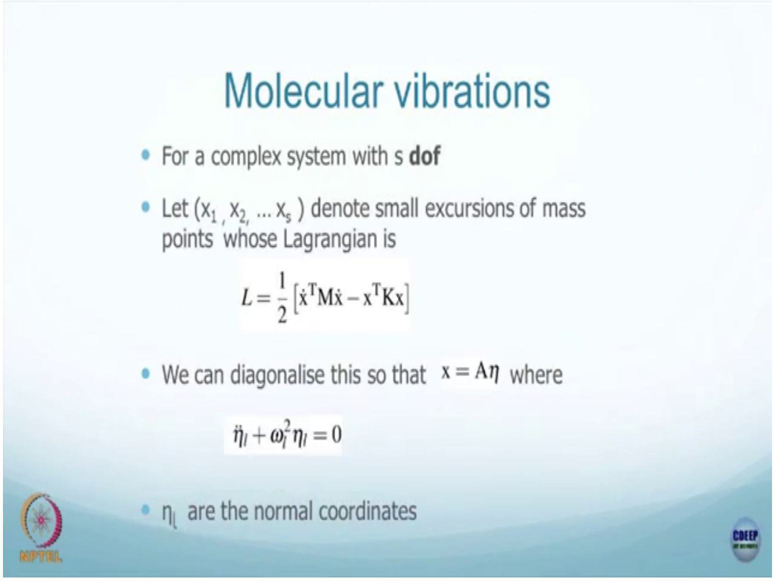

## Molecular vibrations

- For a complex system with s **dof**
- Let ($x_1, x_2, \ldots x_s$) denote small excursions of mass points whose Lagrangian is

$$L = \frac{1}{2}\left[\dot{x}^T M \dot{x} - x^T K x\right]$$

- We can diagonalise this so that $x = A\eta$ where

$$\ddot{\eta}_l + \omega_l^2 \eta_l = 0$$

- $\eta_l$ are the normal coordinates

So, in that case it will be how many vibrational degrees will be there; 3 N minus 5 ok. So, this is what is the theme and for any complex system with s vibrational modes; you can write a Lagrangian involving the slide disturbance away from equilibrium position and you can try an diagonalise such a Lagrangian, right.

M is some matrix which is x cross x matrix, K x another matrix; K has the potential energy; M is the one which incorporates the kinetic energy. So, it is kinetic energy minus a potential energy for a system with complex system or complex molecule; but so many atoms which gives you s vibrational degrees of freedom, right. So, this is the one where you will start finding by diagonalising it, you get your conventional harmonic oscillator; but then L will be s of them and you can determine what are these normal modes, ok.

This I am sure you would have done as an algebra in your classical mechanics. The course here is not to do that algebra, but to get a feel of it from the character table, ok.

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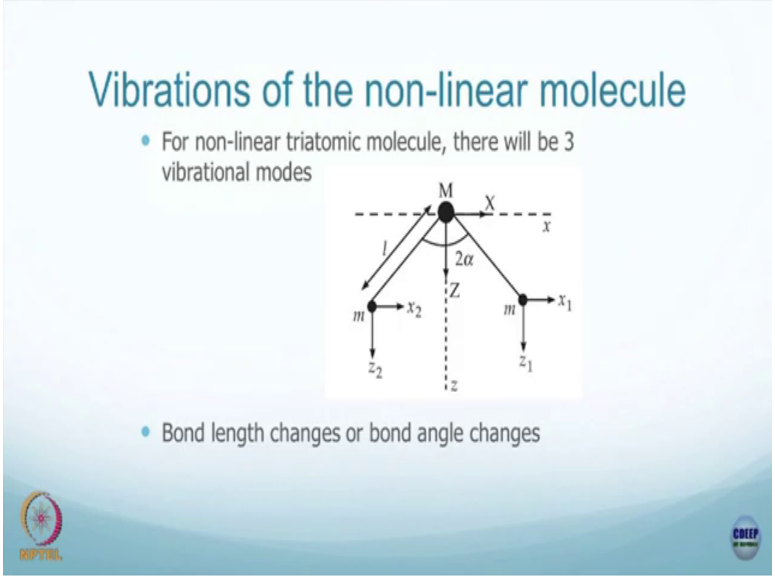

Vibrations of the non-linear molecule

- For non-linear triatomic molecule, there will be 3 vibrational modes

- Bond length changes or bond angle changes

What we cannot get is, we cannot determine the explicit frequencies; but we can determine those normal modes. For example, you take a non-linear triatomic molecule; one of the examples is your water molecule, right. What are the normal coordinates is the question, you can ask.

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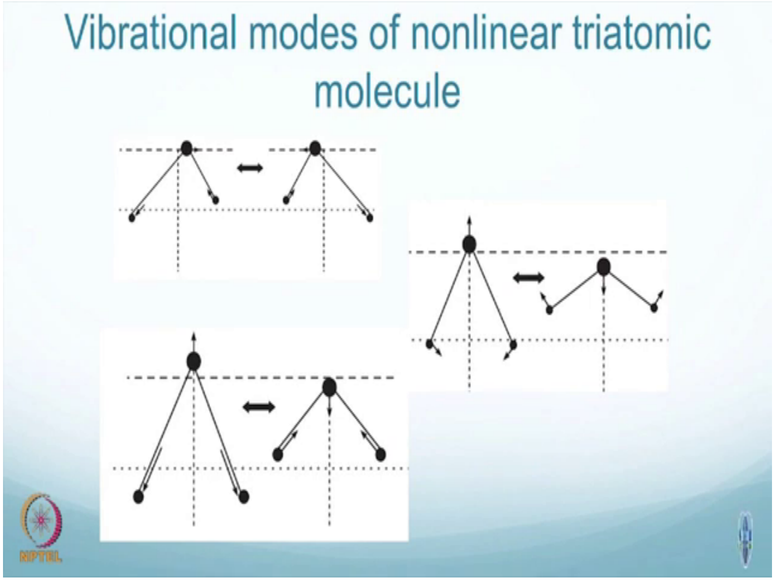

Vibrational modes of nonlinear triatomic molecule

So, the normal coordinates are nothing but this atom is getting disturbed or it moves this way and this atom is moving this way. That is one vibrational mode of vibration, one vibrational mode ok; one normal mode, we call that as a normal mode. There is an equivalent description, instead of doing this even in the two atom thing you do it right; going inside or going outside are nothing but it is a simple harmonic motion. So, these two are equivalent. Other cases a situation where both of them are undergoing stretching; this is asymmetric, this one is symmetric and the third one will be the bond angle can keep changing.

So, you can have these three vibrate; how many modes are there for three non-linear triatomic molecule, 9 minus 6 which is 3 vibrational modes. The three vibrational modes are these objects which have pictorially shown; can we see these pictorially shown objects from our character table, projection operators and get these three objects, ok; so that is the theme and let us end with this 10 minute of video.

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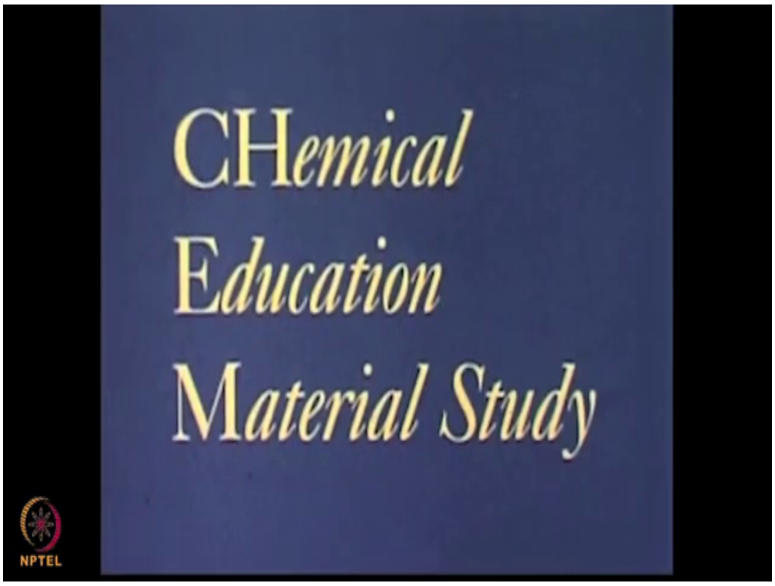

This is a chem study film, for use in the chemical education material study course in chemistry.

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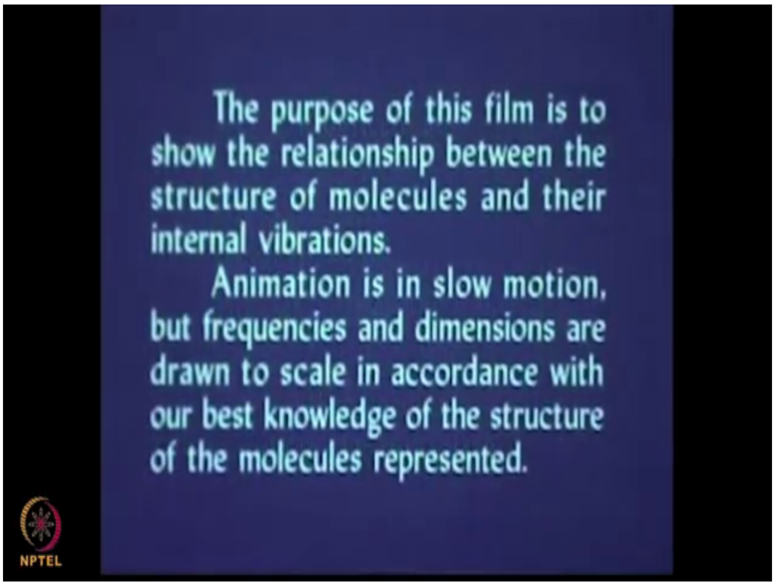

The purpose of this film is to show the relationship between the structure of molecules and their internal vibrations.

Animation is in slow motion, but frequencies and dimensions are drawn to scale in accordance with our best knowledge of the structure of the molecules represented.

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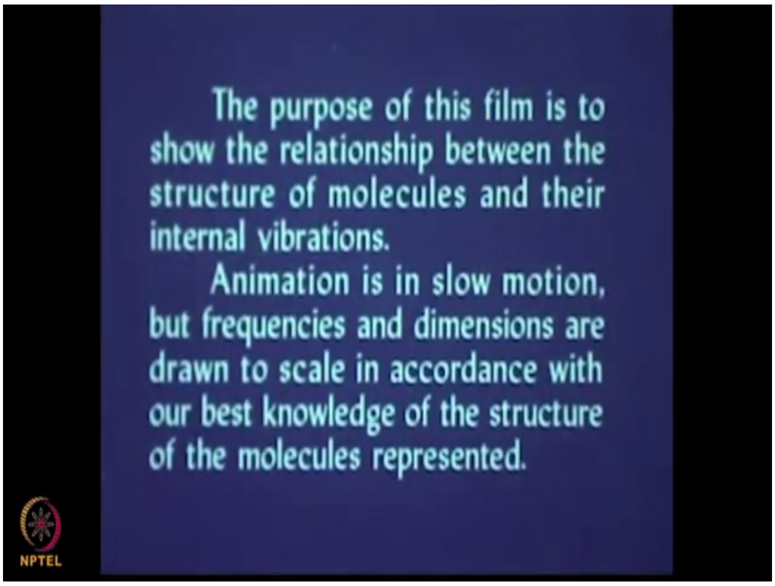

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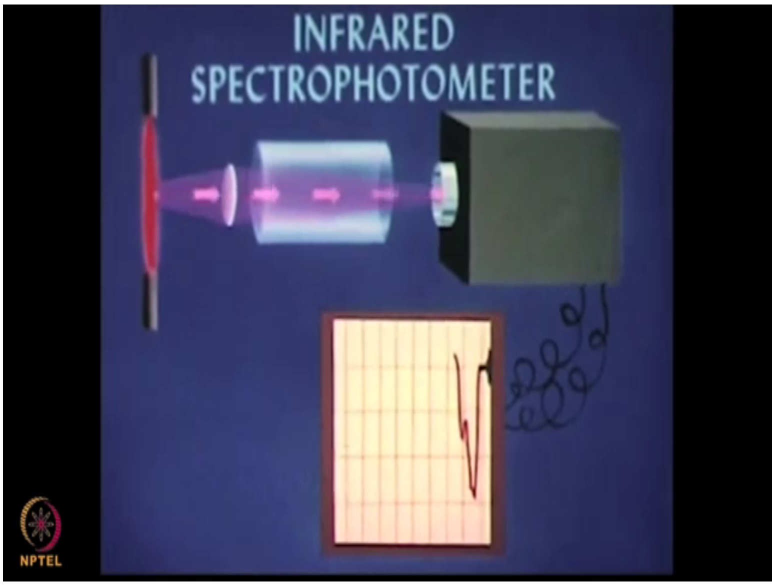
INFRARED SPECTROPHOTOMETER

Molecular vibrations are often studied experimentally with the aid of the infrared spectrophotometer. The molecules of a gas in an absorption cell will absorb certain frequencies from an infrared beam, depending upon their particular structures and modes of vibration. Let us examine a random mixture of gas molecules to gain a better understanding of their movements and structures.

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In slow motion we can see that all these molecules have translational motion. Molecules containing more than one atom can also rotate and vibrate. In this film we consider only vibration, movement which changes the inter nuclear distances.

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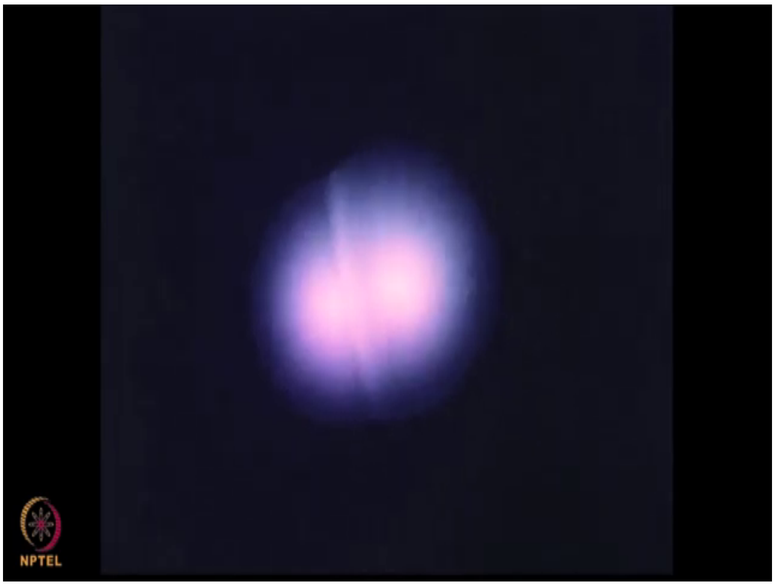

Sometimes vibration is simple and firm as in this diatomic molecule.

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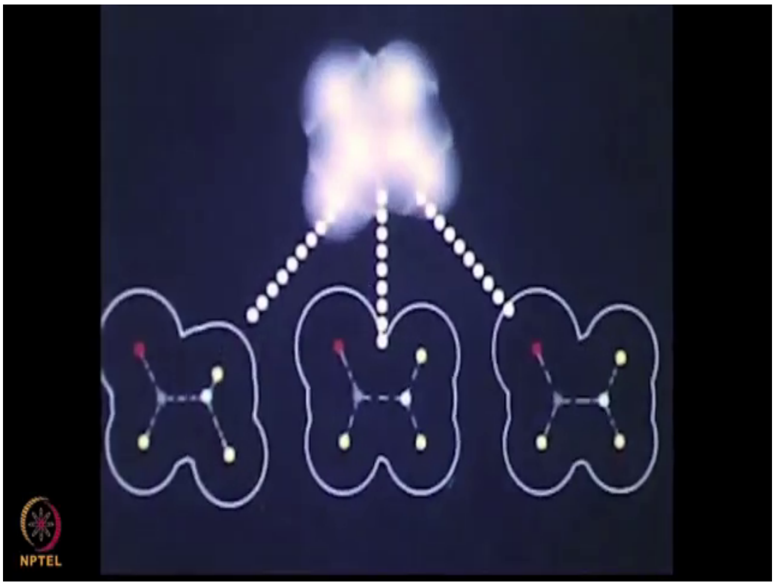

Sometimes as in this formamide molecule it is complex; but what appears here to be a general vibration can be resolved into simpler basic vibrational patterns which are known as the fundamental or normal modes of vibration.

Observing closely some of the normal modes of vibration of the formamide molecule, we can see that each vibrational mode has a different frequency and all of the patterns of vibration may be different. Each of the vibrations is a simple harmonic motion and all of the atoms executing this motion are moving in phase, passing through their center or equilibrium positions at the same instant.

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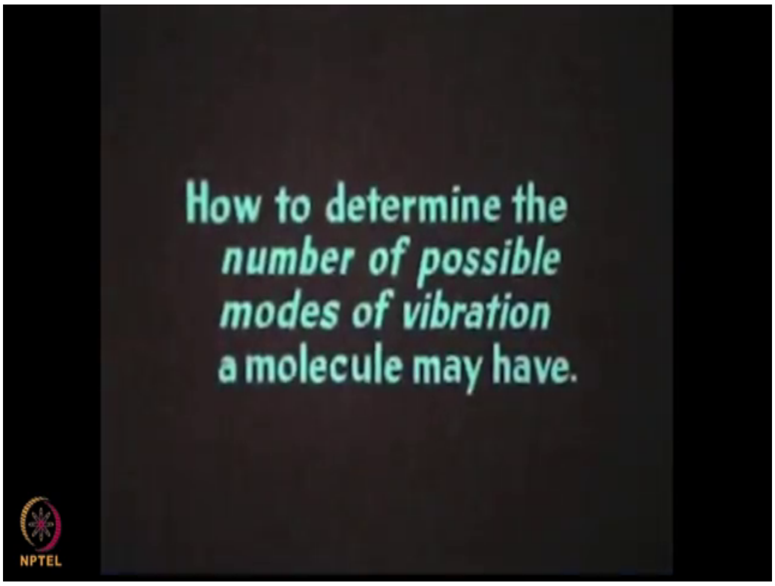

How to determine the *number of possible modes of vibration* a molecule may have.

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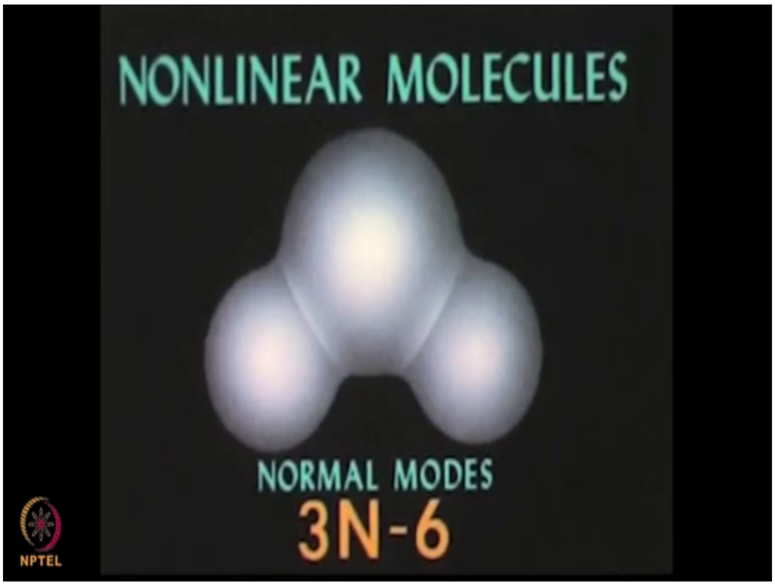

NONLINEAR MOLECULES

NORMAL MODES

3N-6

The number of possible modes of vibration a molecule may have is determined by the number of atoms it has. And for non-linear molecules it is 3 times the number of atoms less 6. Let us see how this result is derived.

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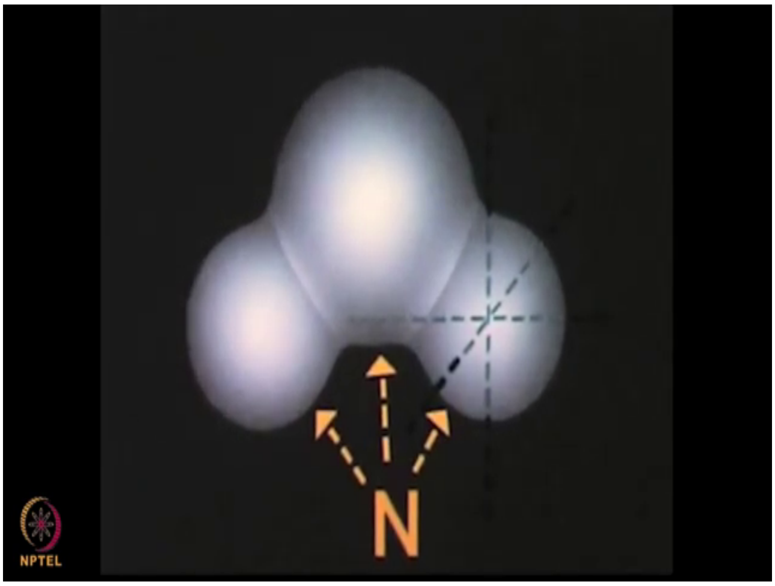

First in order to get the location of an atom in space, it is necessary to specify it is three coordinates.

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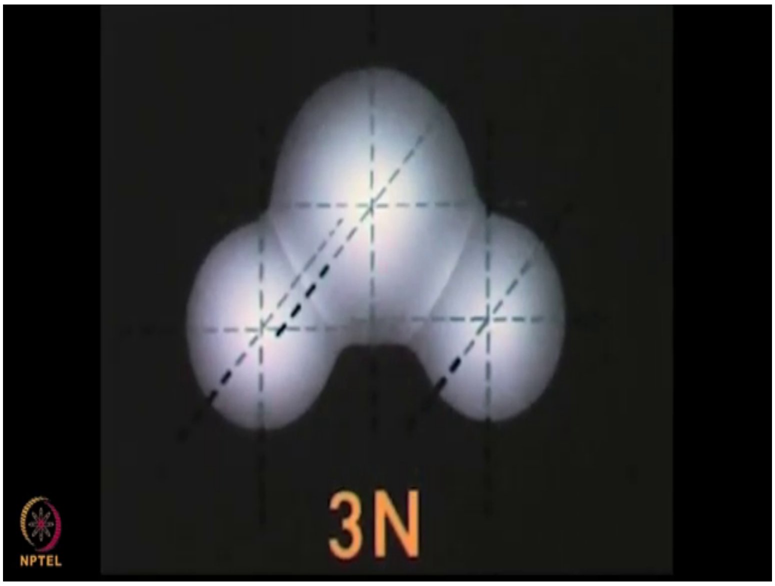

If N represents the number of atoms in a molecule, it follows that a total of 3 times N coordinates are required to specify the positions of all the atoms. There are many ways of designating these positions in space; for our purposes however, we choose a particular set of linear and angular coordinates.

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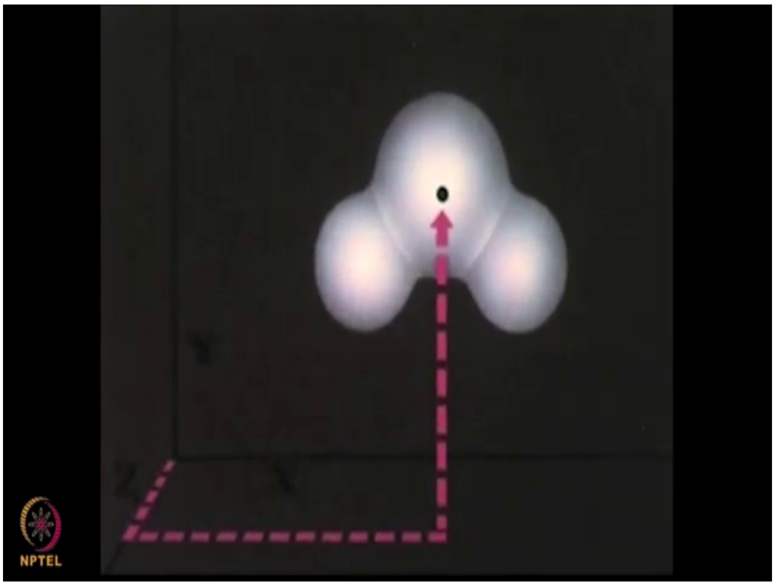

First three of these 3 N coordinates are used to locate the position of the center of mass of the molecule.

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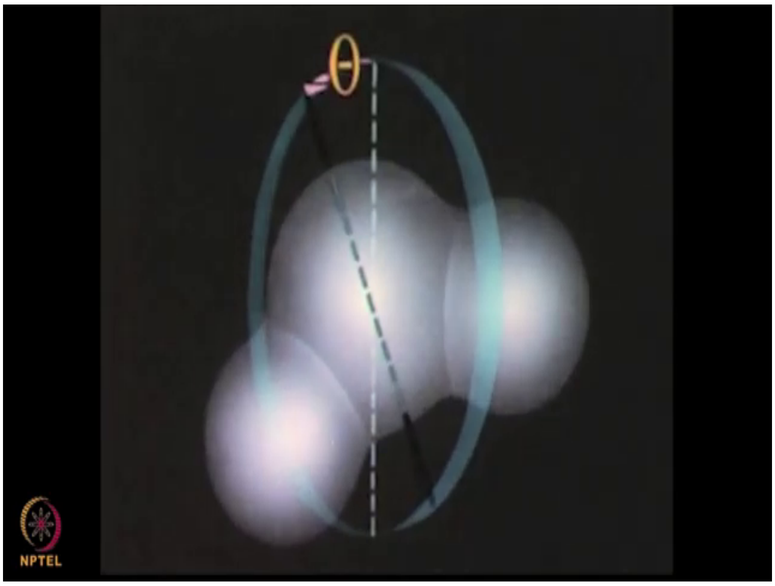

Next we require three angles to specify the orientation of any non-linear molecule. 1.

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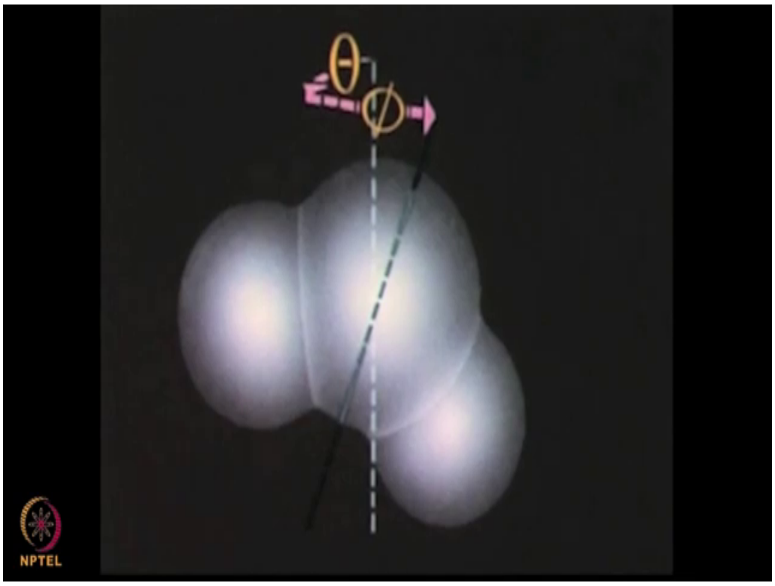

2.

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3.

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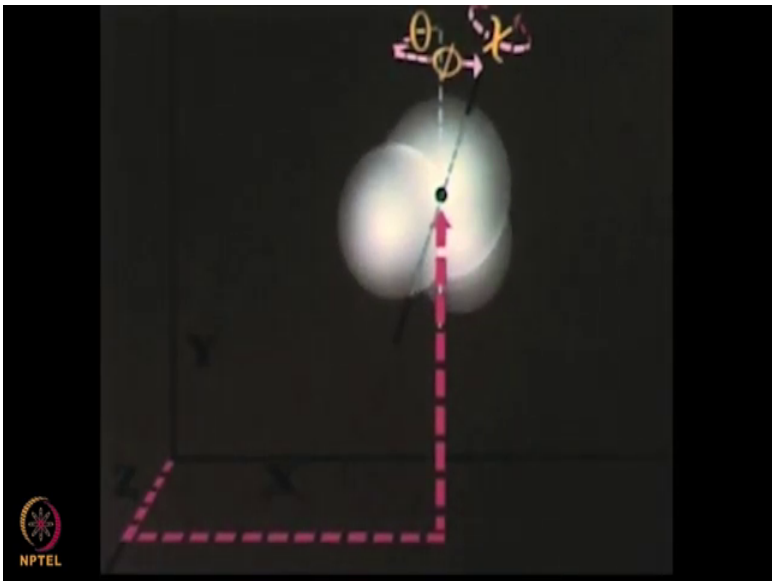

Thus 6 coordinates are needed to establish both the position and orientation of the molecule; 1, 2, 3, 4, 5, 6.

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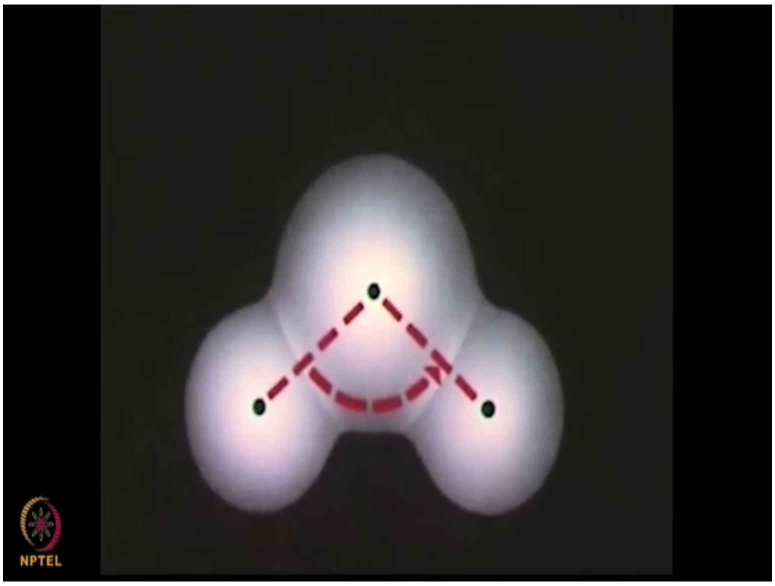

Since we know it takes a total of 3 N coordinates to specify the positions is all it is atoms; the remaining coordinates therefore, locate each atom with respect to the others in the molecule. One such set of internal coordinates in the water molecule includes the two hydrogen oxygen bond lengths and the angle between them.

Now, the positions and orientation of the molecule as well as the relative positions of the atoms within the molecule are continually changing. The total motion may be described in terms of these 3 N coordinates.

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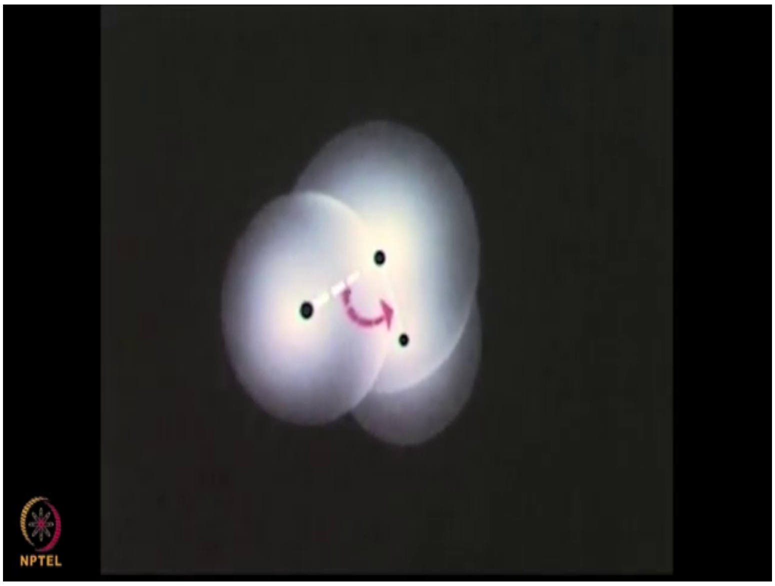

While the internal motion or vibration alone is specified by these 3 N minus 6 coordinates.

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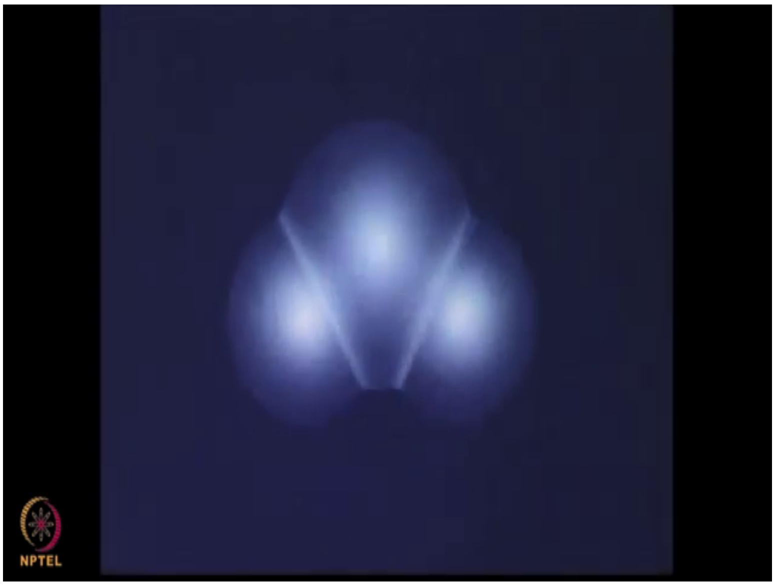

It is possible to find a set of 3 N minus 6 coordinates, such that the complex vibrational motions may be resolved into 3 N minus 6 simple harmonic motions called normal modes of vibration.

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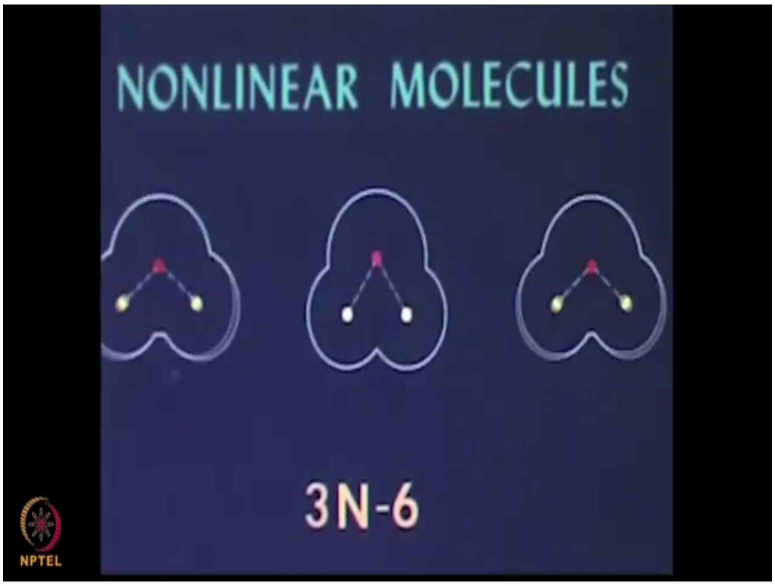
NONLINEAR MOLECULES

3N-6

Therefore, in all non-linear molecules there are 3 N minus 6 normal modes of vibration.

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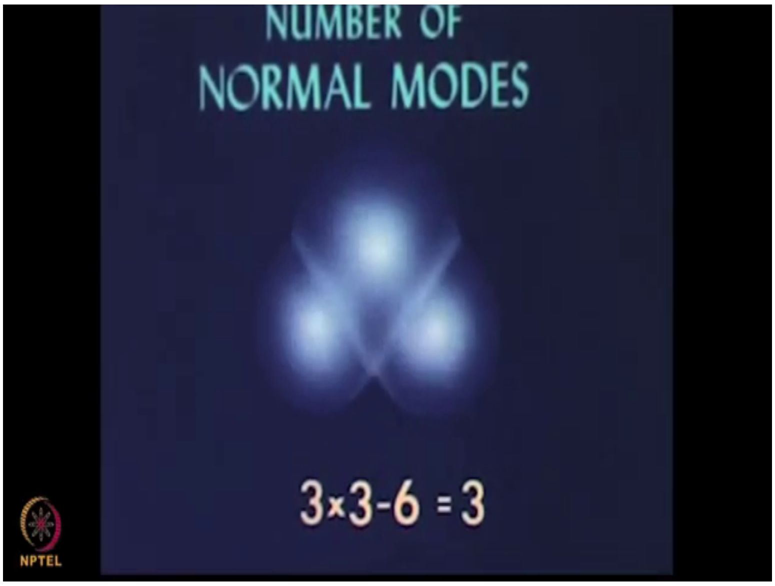

NUMBER OF

NORMAL MODES

$3 \times 3 - 6 = 3$

Since the water molecule contains 3 atoms, it has three normal modes of vibration.

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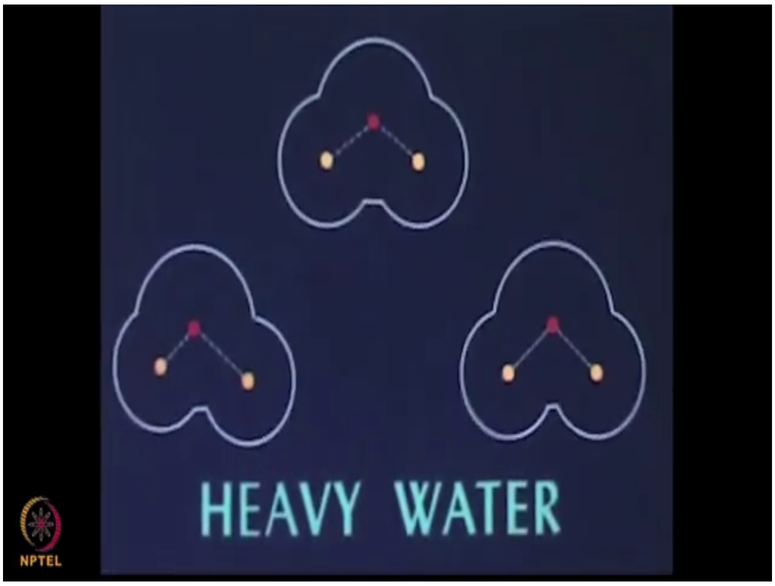

And a symmetric stretching motion, another motion which is symmetric stretching and partly bending of the molecular bond and a third motion which is mostly bending. The frequency of each of these modes of vibration is determined by the masses of the nuclei of the atoms and the strength of the bonds between them. In heavy water for example, the frequencies are lower; because the deuterium atoms have greater mass than the hydrogen atoms.

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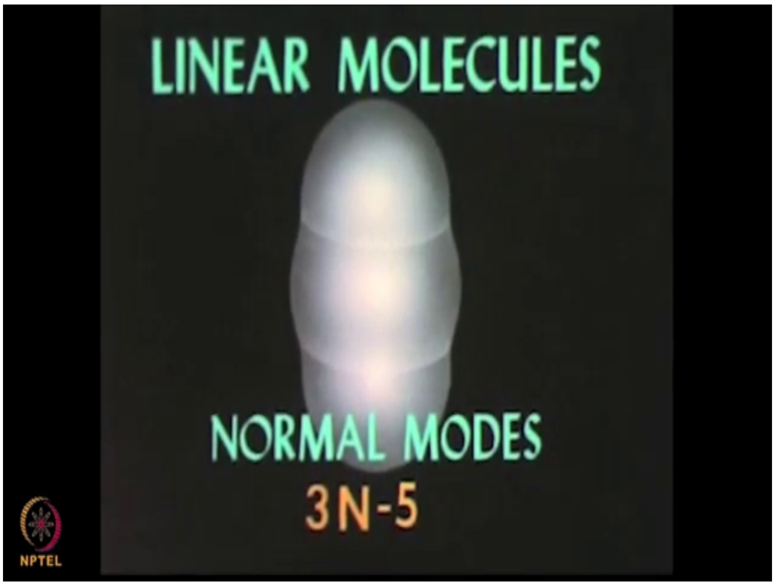

LINEAR MOLECULES

NORMAL MODES

3N-5

For any linear molecule such as this one of carbon dioxide, the formula for the number of normal modes becomes 3 N minus 5; because only two angles are necessary to specify its orientation in space.

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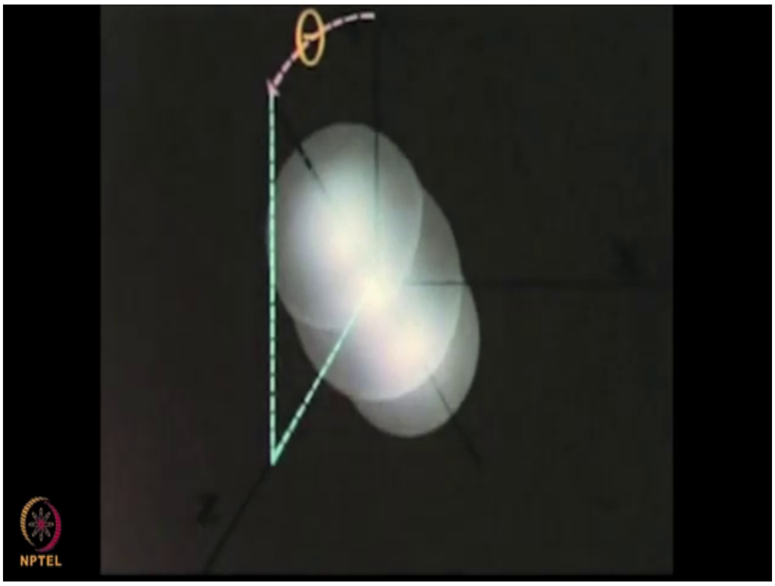

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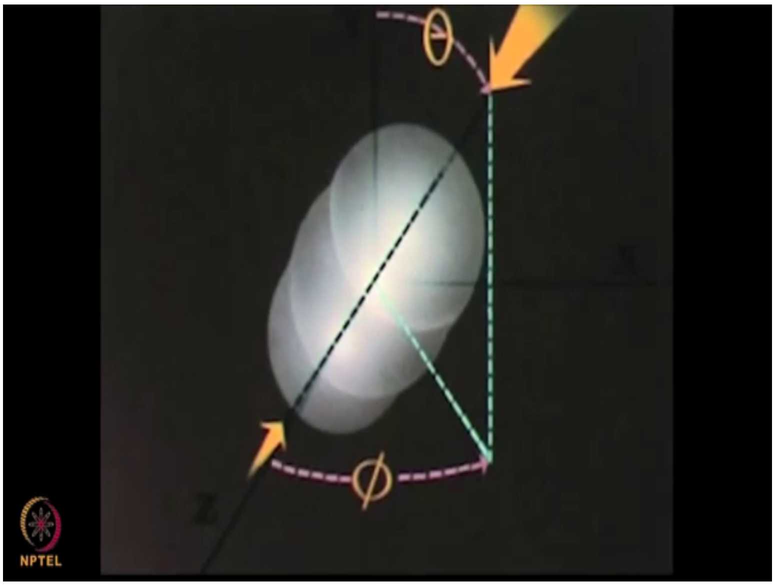

2 The third angle is unnecessary, because neither infrared light nor ordinary collisions impart any rotation around the long axis of a linear molecule.

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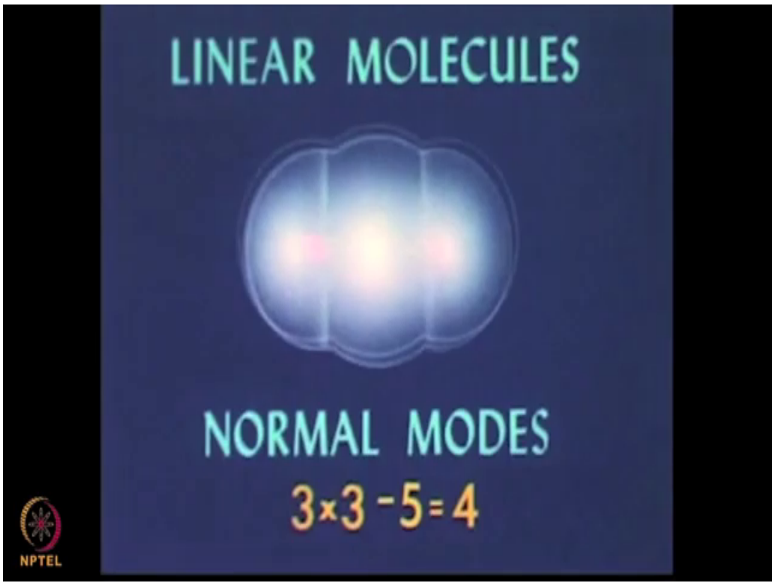

LINEAR MOLECULES

NORMAL MODES

$3 \times 3 - 5 = 4$

This means that the vibrations of carbon dioxide can be resolved into 4 normal modes.

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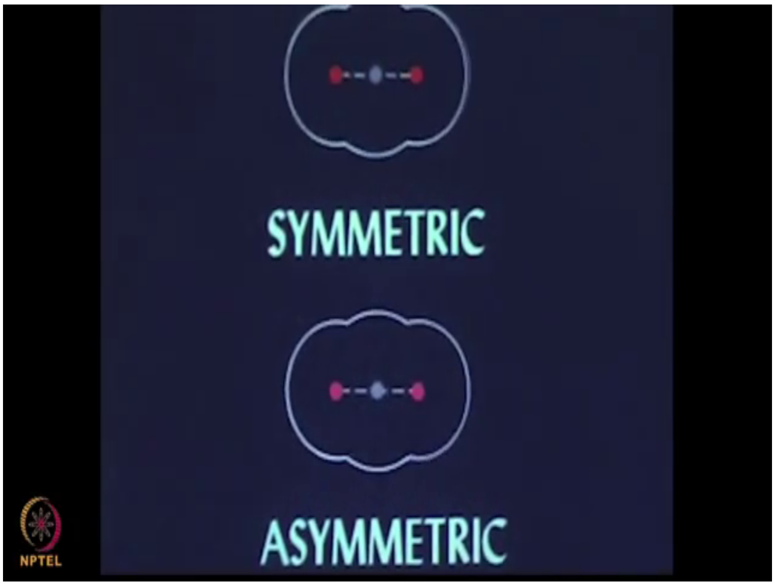

Two stretching modes; a mode which is asymmetric and a mode which is symmetric.

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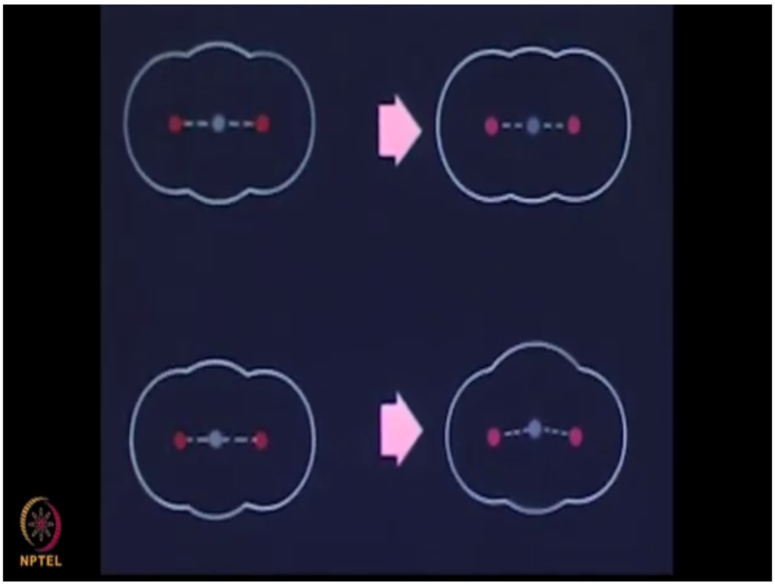

And two bending modes which have the same frequencies, because the same bond strengths and atomic masses are involved. Vibrational modes which do have the same frequency are said to be degenerate. Let us view them from head on.

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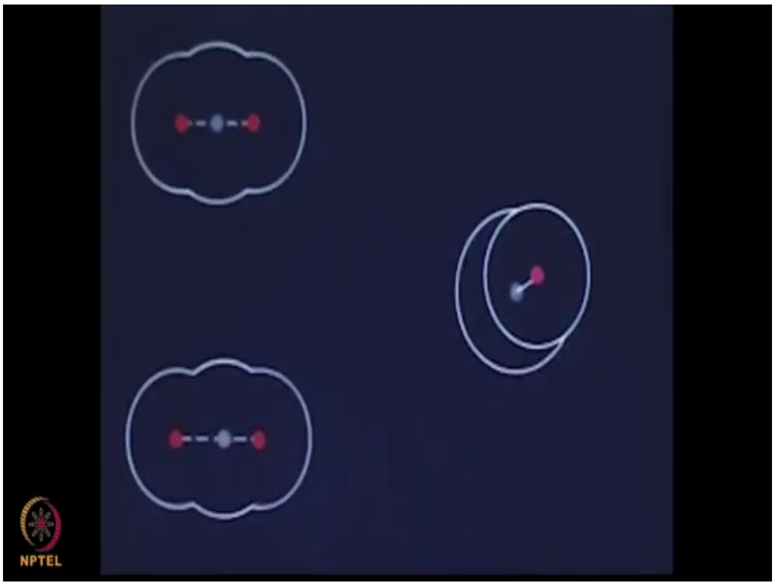

The degenerate modes combined to make a single motion. In this head on view the motion appear is elliptical.

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Next let us examine methane which has five atoms to determine it is modes of vibration. According to the formula, it is vibrations can be resolved into 9 normal modes.

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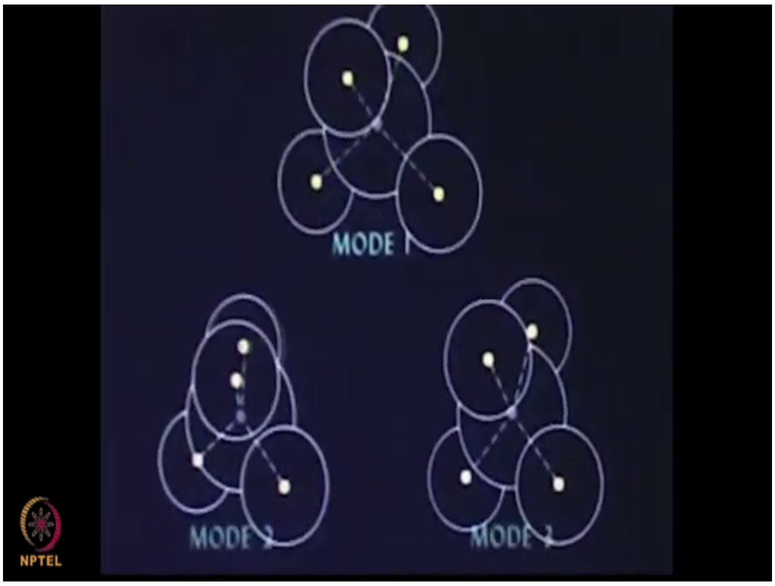

One mode is this totally symmetrical stretching mode also called breathing mode. When we examine it is next two modes of vibration, we find that because of the symmetry of methane their frequencies are the same.

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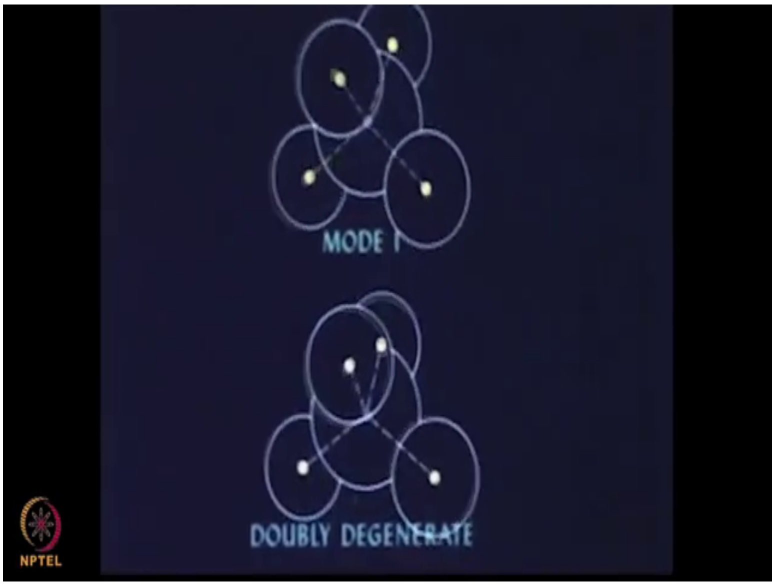

The result is a doubly degenerate bending vibration.

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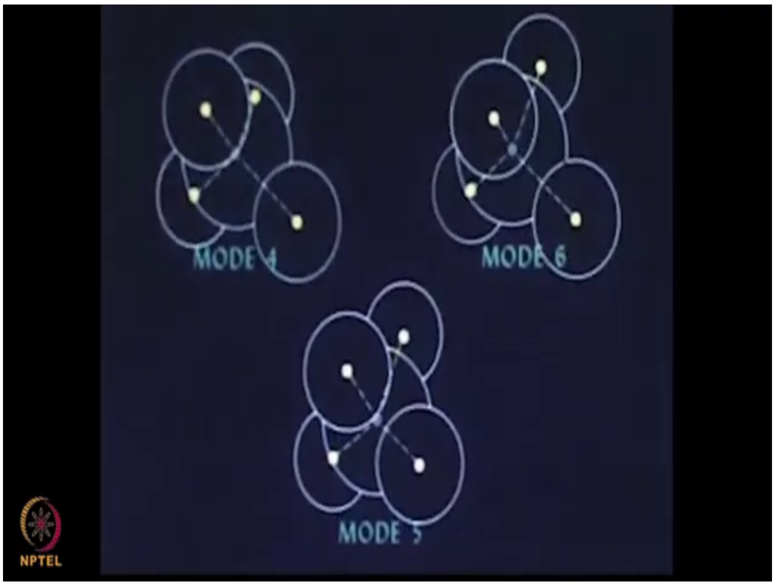

When we look at the next three modes, we find that since the masses and forces are identical.

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These modes combine to give a triply degenerate vibration. This is the asymmetric stretching vibration of methane.

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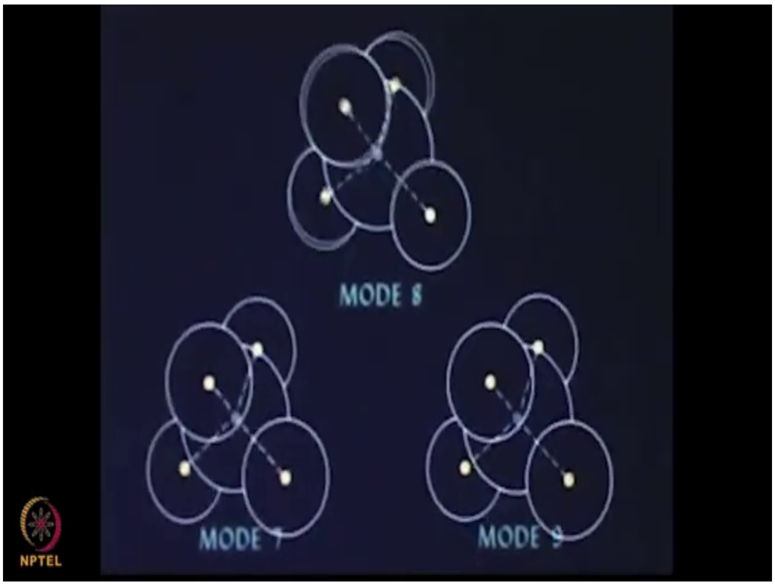

The remaining three modes are also triply degenerate. This is the triply degenerate bending vibration of methane. So, we see that though methane vibrations can be resolved into 9 normal modes, there are only four frequencies of vibration that are different.

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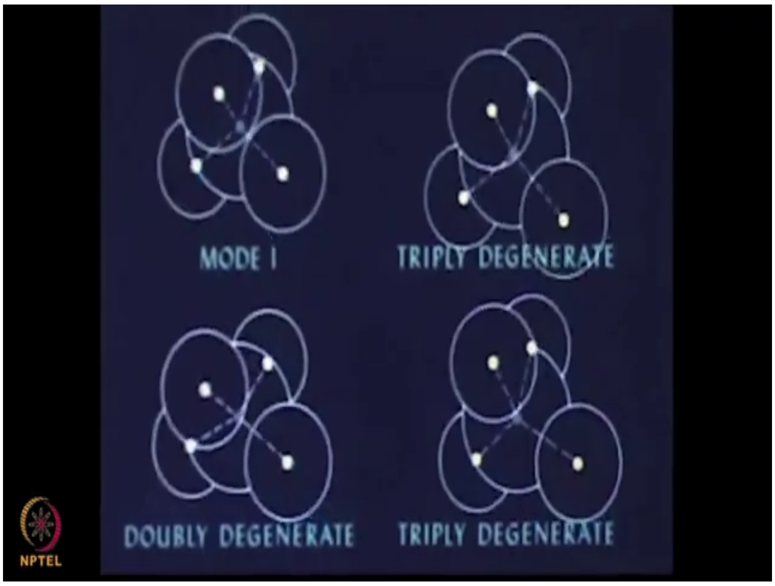

Therefore, methane is a good example of a degenerate system.

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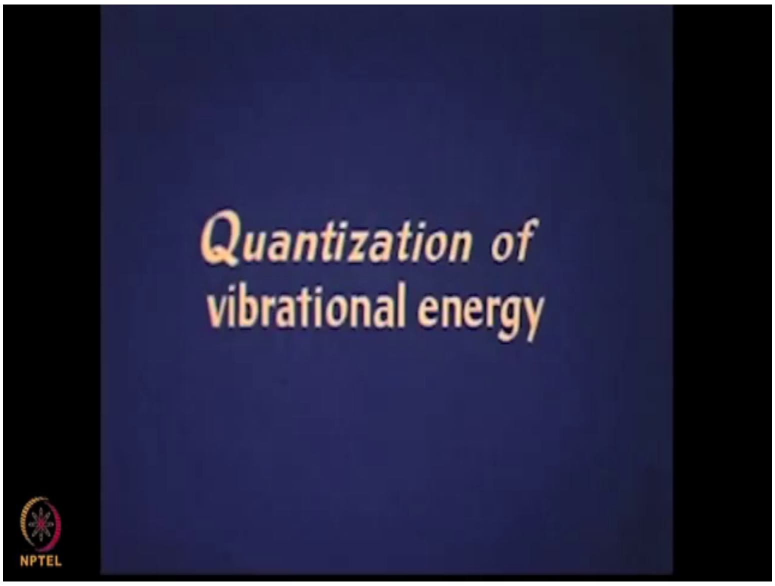

Quantization of
vibrational energy

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A mode of vibration may take on different amplitudes depending on the amount of energy in the molecule. The movement of this carbon monoxide molecule represents it is vibration in its lowest energy state. By collisions this carbon monoxide molecule can be raised to states of higher energy which have the same frequency, but greater amplitudes. By the same means, a molecule can drop back to lower energy states. The same thing can occur through the action of light by absorption or by omission.

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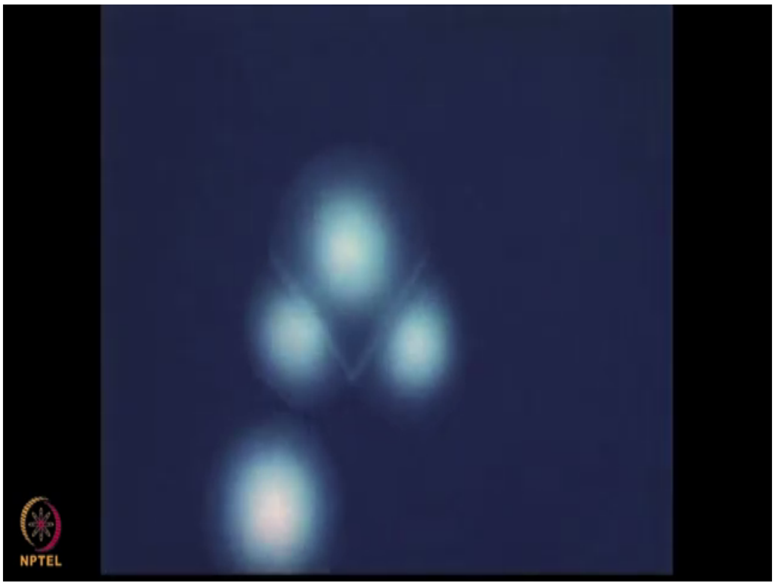

In a polyatomic molecule, water for example; its several vibrational modes may be individually excited or excited in any combination with one another.

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In any molecule the amplitude of vibration increases and also decreases by distinct jumps; because vibrational energy is gained or lost only by definite quanta. Therefore, a molecule can possess only certain discrete levels of energy.

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When a molecule absorbs energy to increase it is vibrational level, it generally absorbs light of the same frequency as one of its normal modes.

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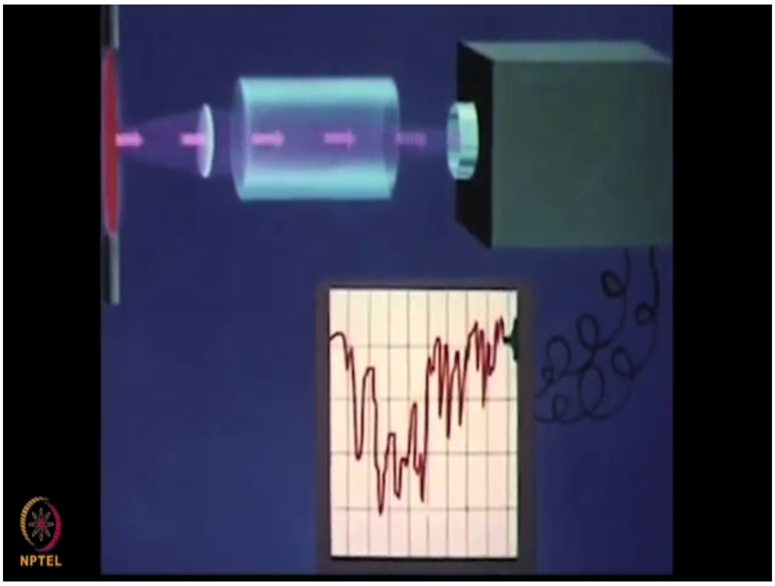

So, by measuring the frequencies of light absorbed, the frequencies of its several normal modes of vibration are measured.

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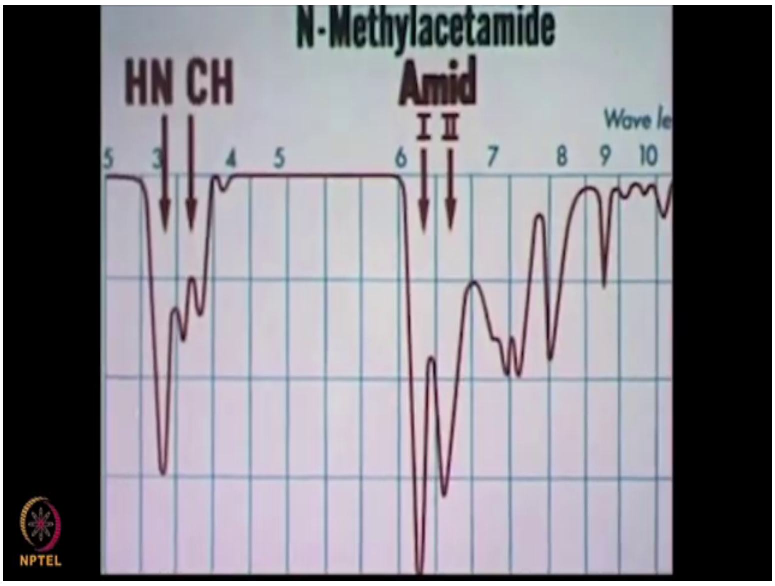

From these vibrations, we derived information regarding energy levels and strengths of chemical bonds. Certain vibrational frequencies are characteristic of certain chemical bonds and serve to reveal their presence in complex molecules. Raman spectra nuclear magnetic resonance and microwaves also reveal the details of molecular structure.

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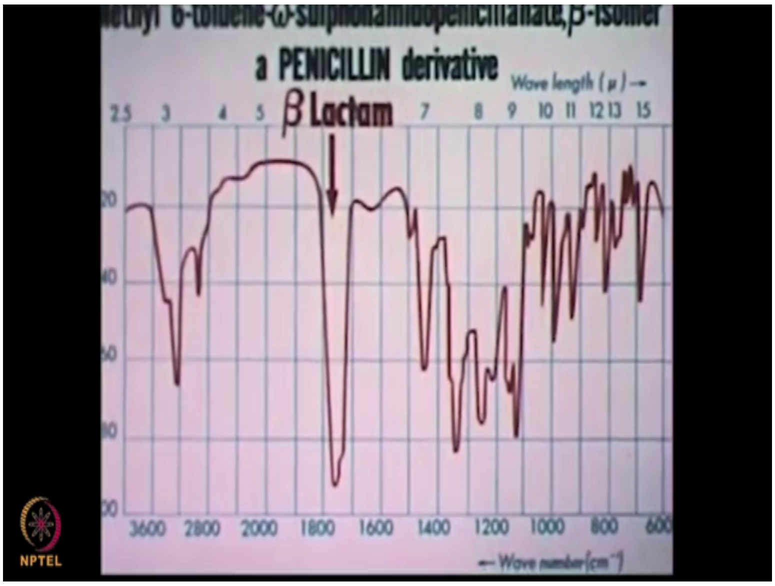

ethyl 6-toluene-ω-sulphonamidopenicillanate,β-isomer

a PENICILLIN derivative

But close to the structure of many important compounds, penicillin for example, have been furnished by the infrared measurement of their molecular vibrations.

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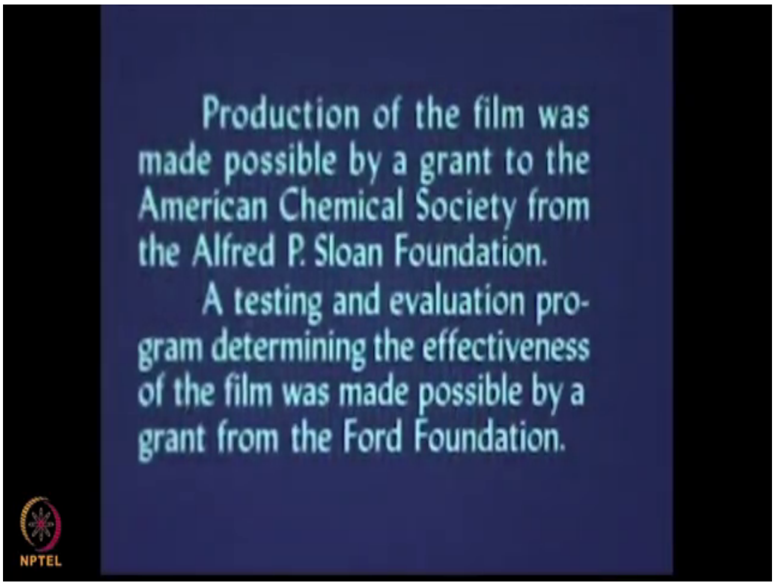

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