Group Theory Methods in Physics
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Lecture – 13
Symmetries of Molecule, Stereographic Projection

So, let me try to give you a flavor of how to see these groups in a method called Stereographic Projection. I am sure everybody would have heard about stereographic projection. You can map things on the 3D onto the 2-dimensional plane right, you can do this mapping.

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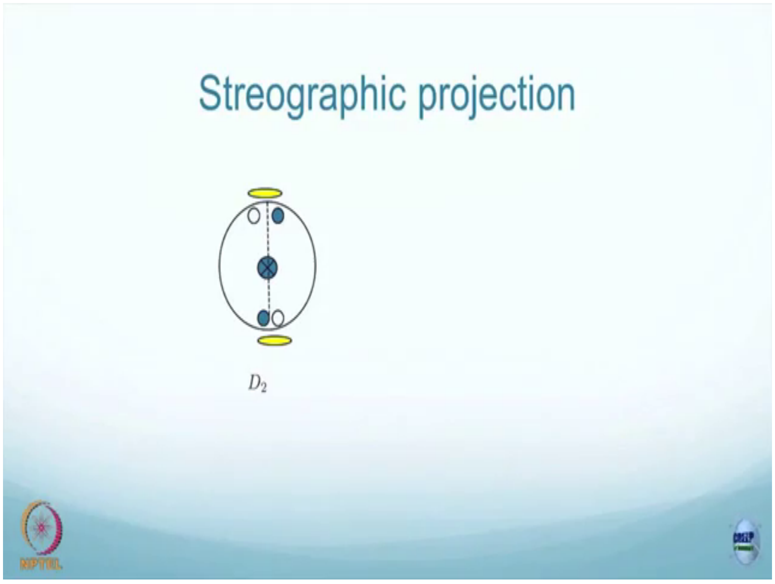

And, what we are going to use is that, the thing is, we put the molecule first to start with; let us take one of the atoms of the molecule here and when I do the C 2 say I am going to just concentrate on one atom of the molecule and I will do a C 2 operation ok. So, when I do a C 2 operation and draw it on this plane, this atom will move to this.

So, the claim is that if there is a molecule with both the atoms at these two positions it will be the symmetry C 2 will be the symmetry of that molecule with two atoms and the point group will have two elements also ok. So, now, let us go to C 2v. C 2v start with the atom you do a rotation. So, then you do the reflection. If you do a reflection you end up getting four atoms ok. So, this is one way of saying that the symmetry C 2v starting on one point you can generate all the four elements of that point group C 2 ok.

So, same way you can do it for dihedral group. I have taken the simplest case we can do for complicated case. So, take the dihedral group, as I said you have a principle axis here. Now, this principle axis is also C 2 and then you have an axis in the which I am shown by a dotted line and with these two hats put on it to say that this is an axis which is perpendicular to the principal axis and you start. You take a point.

When you do a C 2 rotation it goes here; when you do a D 2 rotation what will happen? It goes behind; it goes behind the plane unlike your mirror reflection behind the plane I showed by a hollow circle. So, this symmetry is not going to be the symmetry of a water molecule ok. So, this is slightly different it goes behind the.

Student: (Refer Time: 03:09).

Huh.

Student: (Refer Time: 03:12).

I am not able to hear you.

Student: It involves (Refer Time: 03:15).

That is right ok.

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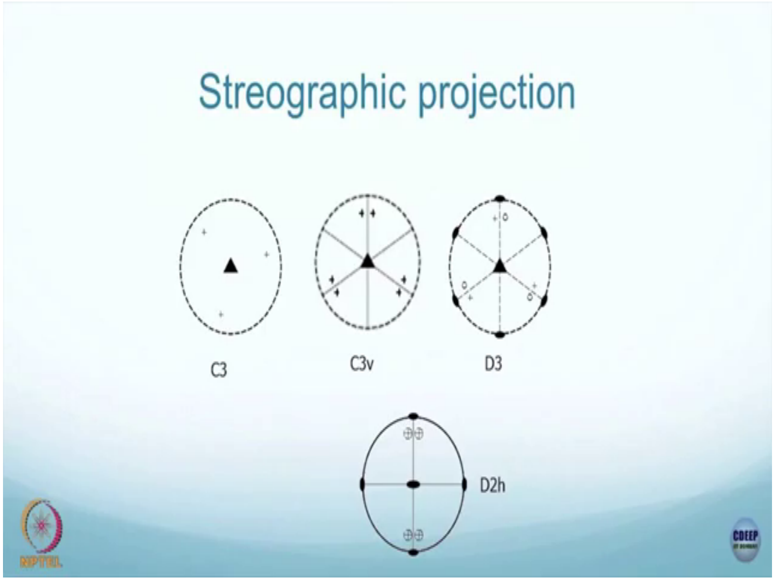

So, just to show you more C 3 I can put these three hydrogen atoms here ok. If you take C 3v then by mirror reflections you can have one more element added here this way; if you do D 3, it is this ok. If you do D 2h what happens? Every element you have to do a mirror reflection on the xy plane, object in front of you goes behind you. So, that is why you have both plus and minus your plus and plus is for the filled circle and circle is the hollow circles I put both together.

Here if you see I do a C 3 rotation so, the plus goes here, plus goes here and then I do a sigma v reflection which means you will have sorry not sigma v this is the 2-fold axes rotation. So, you will see that this element goes here and then this element goes here and so on. This is clear to you?

Student: (Refer Time: 06:39)?

So, D operation is we over on top of this 2 f pi by n rotation you do a rotation about an axis perpendicular to the this axis, that is all ok. So, if you take the ammonia molecule so, D 3 will involve E C 3 C 3 squared and then you will have a u 2 you will have a C 3 u 2 and C 3 squared u ok.

So, these three things you can see as if it is the to start with you had 1 2-fold axes just like in your ammonia molecule to start with you add one mirror plane, but then the other elements can be seen as new mirror planes right. Similarly, you can see this as u 2, u 2 prime, u 2 double prime as 3 2-fold axis, but all of them are in the xy plane and they will be perpendicular to the z axis.

So, that is the D 3. And, in this notation D 3 will correspond to n equal to 3. So, what is your confusion? Now, it is clear ok? Any doubts on the stereographic projection?

Student: Mam.

Yeah.

Student: (Refer Time: 06:11).

C 3v. So, let us do it maybe that will clarify for you.

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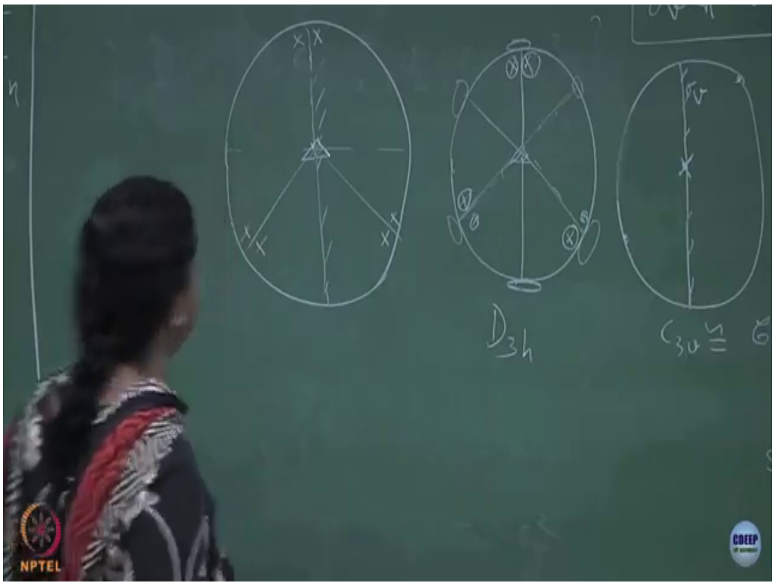

So, you have the axis which is the 3-fold axis of rotation which is sometimes denoted universally as a triangular point at the center and then you take either a filled circle or call it as a cross. If you do a; if you do a 120 degree rotation this one has to go here ok. If you do a 120 degree rotation of this then this one has to go here and if I put a mirror plane on this object when I put a mirror should give me another one which is here on the same plane.

Student: (Refer Slide Time: 07:24).

Mirror plane has to be with this it should be the as I said you start with some conventional mirror plane you could put it along this also you have to put it on the plane of symmetry. These three atoms if it has a C 3 symmetry I cannot put mirror like this that is what you are asking. If I put it here then this will give you completely different things know. So, if I am generating a C 3v symmetry I make sure my mirrors are not arbitrary in the xy plane.

Student: (Refer Time: 08:07) mirror planes pass through the.

Pass through the.

Student: (Refer Time: 08:09).

So that you get back your elements back right. So, if I have this mirror plane this element will go here, this element will go here and this element will go here.

Student: (Refer Time: 08:27).

Mirror plane is.

Student: Is not passing through one of the you know this.

I am not able to hear you one of the; one of the I am hearing.

Student: (Refer Time: 08:40) passing through (Refer Time: 08:44).

So, the way you should view is that I have projected it you can view this as if it is a spherical atom and the left region gets mapped to the right region in some sense that is another way of using ok. So, here I am doing a 2D projection that is why it is called stereographic projection. And, the C 3v symmetry when you are doing it technically this atom goes into this atom is what you would have looked into it, but as a point a group element there are six elements in the point loop to see that we explicitly put it as if there are points and how it transforms under a C 3v symmetry ok. This is all I am saying.

Any other confusion? And, similarly D 3; D 3 will also have the symmetry, but then you will also have a 2-fold axis symmetry and then you start generating this one will go behind when you do a D 2 rotation and similarly this one is because of this one going here and this one will go here ok. And, equivalently as a plains of symmetries after you have drawn the stereographic projection you can see that there is one plane which passes through this sorry, not plane D 2 axis.

This is D 2 axis, this was one D 2 axis and this one will be another D 2 axis. Is that clear? There will be three D 2 axis. If you ask a chemist what are the symmetries they look at symmetry planes and symmetry axis, he will say that there are three axis 2-fold axis which are passing through each of the atoms and then he will say that there is also a 3-fold symmetry that is what he will say for a D 3.

If you ask him for a C 3v molecule he will say that it is three mirror planes and one 3-fold axis rotation ok. To him he will only look at this axis of symmetry and planes of symmetry, is that clear?

Student: Maam.

Yeah?

Student: (Refer Time: 11:36).

With ppt the last one D 2h?

Student: Yeah.

So, if you do a D 2h so, let us look at D 2h also anyway you can also do the D 3h. So, this is D 3 if you want to do D 3h you also have a mirror on the xy plane. So, when you have a mirror this cross will go behind also the behind one will come up and so on. So, that will be the. So, in fact, looking at these points you should know how many elements are there in D 3h. So, D 3h will have how many elements?

Student: 12.

12 elements ok. So, that is the way you can also look at a glance and get a feel of these point groups. Now, I am not looking at any specific molecule I am trying to generate all the elements of the set of the point group by putting in the axis of symmetry and the plane of symmetry to start with. I make sure that I start with axis of symmetry through the center of this stereographic projection plane and plane or axis of or the 2-fold axis symmetry to be something which is coinciding with or perpendicular to this.

The plane coincides contains the principal axis or I am looking at a 2-fold axis perpendicular to the principal axis. And, then the other principal axis and all gets generated, but they can also be viewed as compositions of sigma v times C 3 else more. Is that clear? These are various equivalent ways of interpreting the group elements of a finite group in the language of symmetries axis and symmetry axis and symmetry planes of a molecule.

So, I have just given it on the slide a D 2h plane ok. In the process of doing it you can see that these are equivalently you can. So, looking at this point group thing a person will say there is a 3-fold axis symmetry and then one 2-fold axis, second 2-fold and third 2-fold. And, here it will be like you will have 1 2-fold axis at the center because it is D 2 and then you have one and another 1 2 2 2-fold perpendicular to it, clear.

And, also in the picture whenever you have a sigma h plane they replace that dotted outside circle by a hard circle ok. So, looking at it they should know what is the symmetry group they are looking at it. So, once they see a solid circle they will know there is a sigma h symmetry and then they look at all these points and these axis which are shown here and they will know what are the elementary operations which are there.

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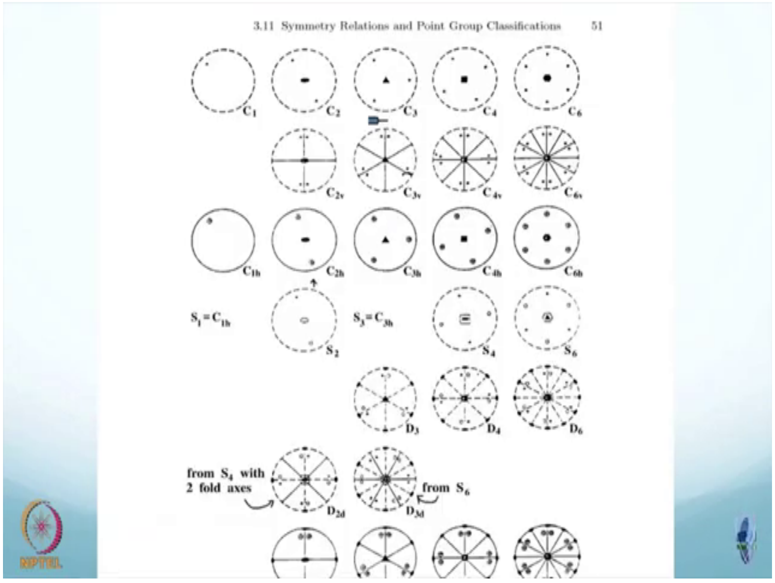

So, any book if you take it will all be there you can go and look at any book this whole like a periodic table or you know. It is not specific to an atom or it is specific to a molecule, but generally point groups are shown in this shorthand notations. You can see if I write C 4h C 4h has a 4-fold axis and then the outside circle is solid circle, is that clear?

So, these are all rotoreflection. Now, you do rotoreflection here. If you do rotoreflection what will happen? It is 2 S 4 S 4 if you want to do it tell me how it will be? So, you have a cross here. The cross rotation you would have made it cross, but I have to do a reflection about a plane. So, it will become backside and again if I do a 4-fold rotation it will come in the front and then again I do it will go to the back.

So, the rotoreflection is nothing, but C 4 times sigma h and clearly you can see the diagram is not isomorphic to C 4 you can never make it isomorphic to C 4 right. It has an improper component. But, can we do the order reversed? Can you do first sigma h and then a C 4? If you do a sigma h on this it will go behind and then you do a C 4 it will be here. So, in fact, this is going to be sigma h C 4. So, S 4 will also be an Abelian group ok. So, ways of seeing it from the diagram, is this clear ok?

So, those are the notations which are given here and you can show that there is no distinction between S 3 and C 3h ok. C 3h whatever you have drawn here if you draw S 3 it will be exactly similar to C 3h, please check it out ok. And, S 4 I have already drawn for you; S 6 again will be similar, but 6-fold axis symmetry and D 3 I have already discussed. And, then you can also have diagonals planes which is what is being discussed here ok. So, I leave it you to check some of these things and play around a bit ok.

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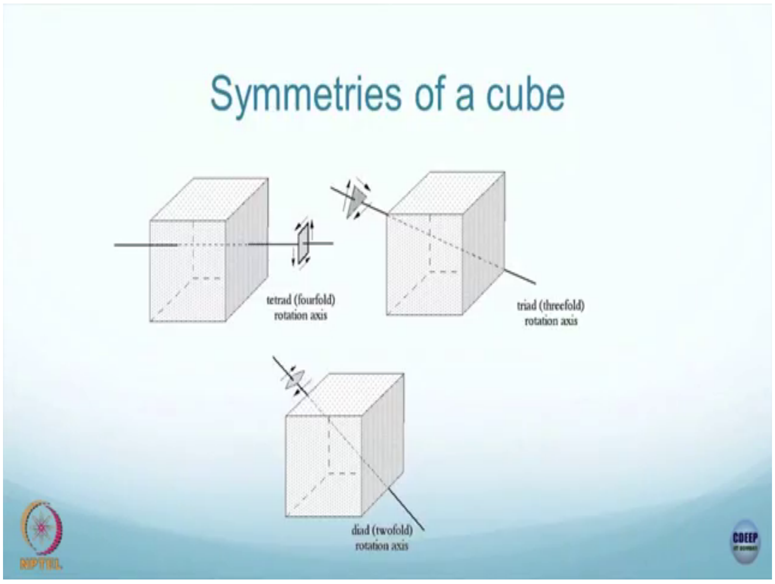

So, this I have already told you that some molecules with cubic symmetries can be present.

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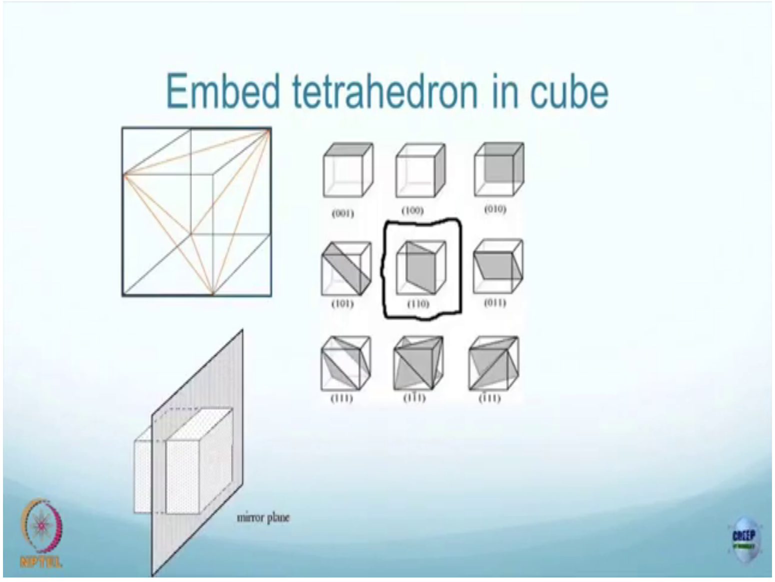

Some molecules can have tetrahedral symmetry, but tetrahedron can be also seen by embedding inside the cube ok.

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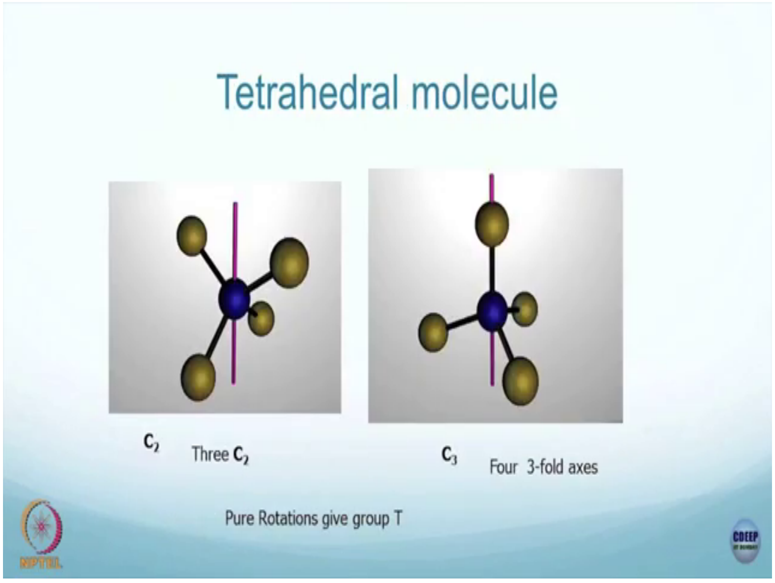

So, just to give you a flavor of the tetrahedral molecule I am just taking one or two examples to motivate you. Anybody is like into this you should go and list all the molecules and look at how things are. In fact, they have these kinds of animation where you can see the axis of symmetries and planes of symmetries of the molecules ok.

So, if you take this, this is the methane molecule you can take it to be the methane molecule with the 4 hydrogen and centre blue one is the carbon and then these are the C 2 axis rotations. And, there are three C 2 axis and there are four 3-fold axis each 3-fold axis is going between one hydrogen and carbon C-H bond ok. Oops, I thought the animation will come here. It will not?

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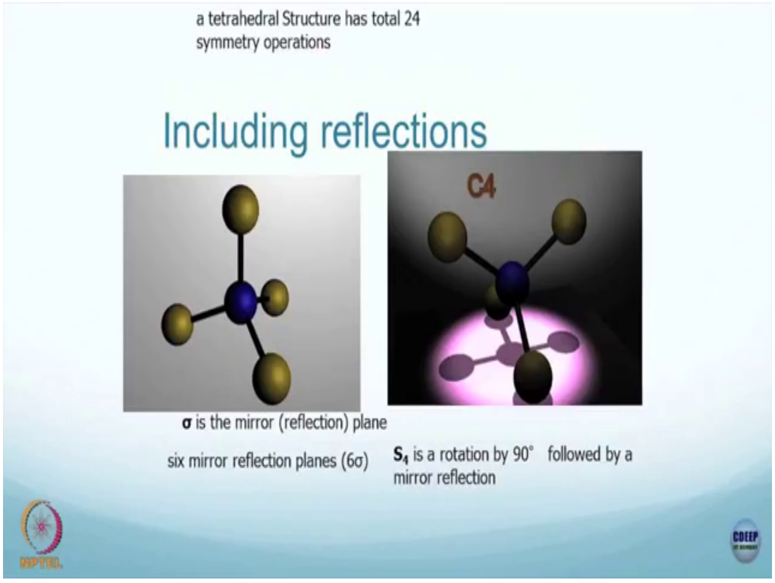

I had the animation also. Unfortunately, it is not coming here ok. So, see some of these molecules have this rotoreflections ok. Rotoreflection is S 4 especially this methane molecule has an extended symmetry which involves sigma plane, mirror plane. There are six mirror planes and leave it you to check these things I had this animation which was supposed to show you that.

Here rotoreflection what happens is that first you do a rotation it does not go to the configuration. But, you have to do a reflection on this plane and then it goes into the configuration. So, it is very beautiful.

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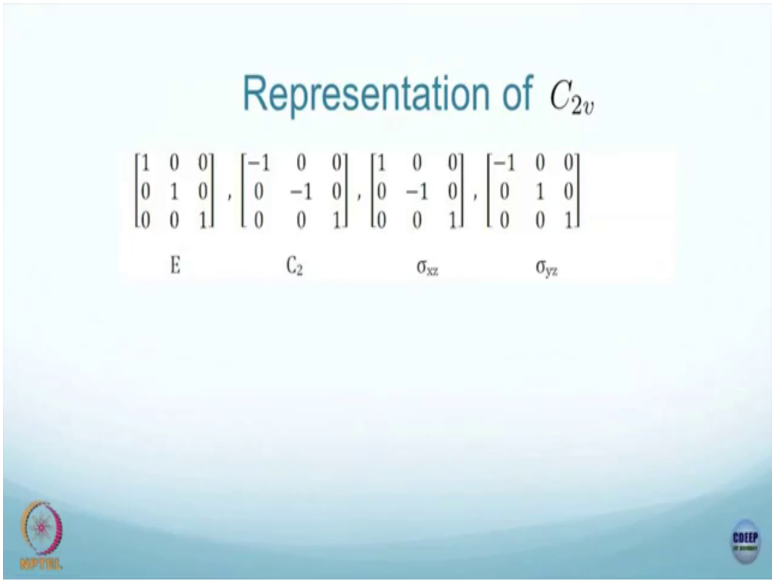

So far what have we done? I have tried to give you a flavor of point groups and these point groups are again finite groups and they can be shown to be isomorphic to subgroups of symmetric group of degree n ok. And, I have introduced what are the fundamental operations with which you generate those finite point groups either rotation axis, reflection axis and axis perpendicular to the principal axis and whenever you have an axis perpendicular to the principal axis then you can show that C and C n, C n k and C n n minus k will be conjugates to each other.

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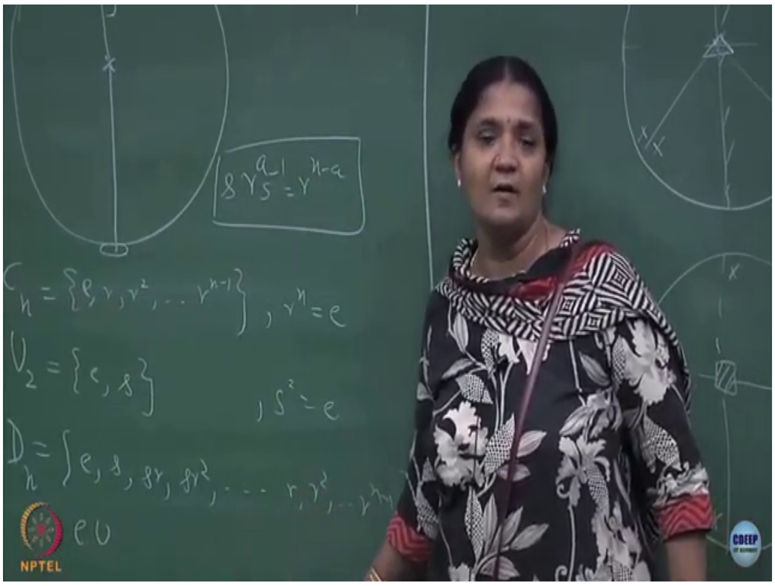

And, similarly even if you have a mirror plane containing the axis principal axis then you can show that these are conjugates to each other. And, I have left you to try and understand the conjugacy classes of the dihedral group and similarly the conjugacy classes of the C n v group ok; when n is odd, when n is even what is happening you have seen that the rotoreflection group is a Abelian group.

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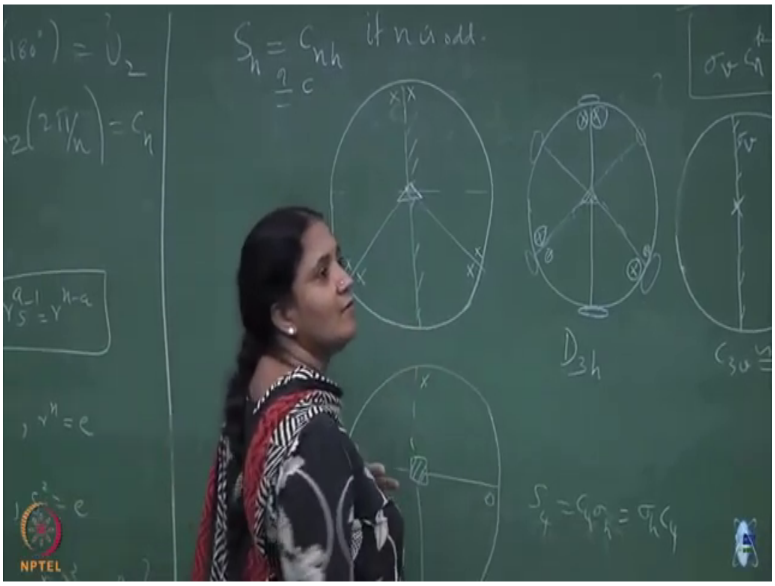

And, you can also show that the rotoreflection S n is not very different if n is odd ok. So, you can try and check it out do S 3 rotoreflection and do C n h and see whether there are any distinctions ok. So, these are things which I want you to get to feel about some of these by playing on the stereographic projections and understanding whether this is true is this true or is this true you know I leave it you to check all these things ok.

And, the next thing which we are going to take up is to give matrix representations to all these point groups ok. For example, if you take C 2v; C 2v is a point group you can write matrices in your xyz basis right all of you know that. Identity element is nothing, but the unit operator right and C 2; C 2 is 180 degree rotation which will change x to minus x, y to minus y. So, the matrix will be having minus 1 minus 1 in the first two and then they will C 2 will z axis is unchanged.

Sigma xz will change y coordinate to minus y coordinate, xz will unchanged and reflection in the yz plane will change x to minus x, yz will be unchanged. So, this is what we will call it as a matrix representation for the same C 2v group; C 2v you can write a multiplication table. The same multiplication table will be satisfied by the matrices right.

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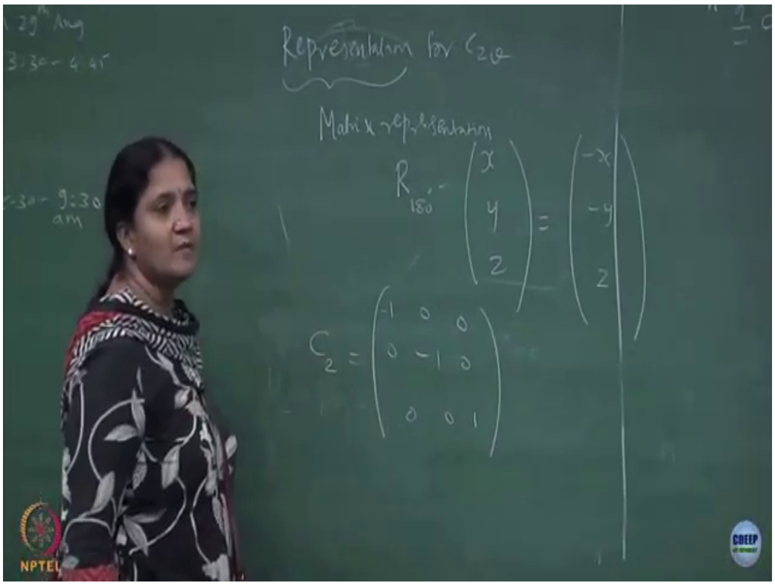

So, we give a representation. So, specially the representation which we are going to look at is matrix representation, because one is that we can do the composition the group operation as multiplication and you also know that how you can operate it on vector spaces. Suppose, this one is the 3 cross 3 matrix you can treat this matrix to be operating on a space which has x, y, z coordinate right and you can you know what this answer will be.

Suppose, it is the rotation by 180 degrees right you know the answer has to be minus x, minus y and z I am right? No. Is that right? Yes or no? And, what is the matrix which can generate that state? If you try to find then you know it is minus 1, 0, 0 ok. So, this is what we will call it as a C 2 element and similarly, all the other elements can be written.

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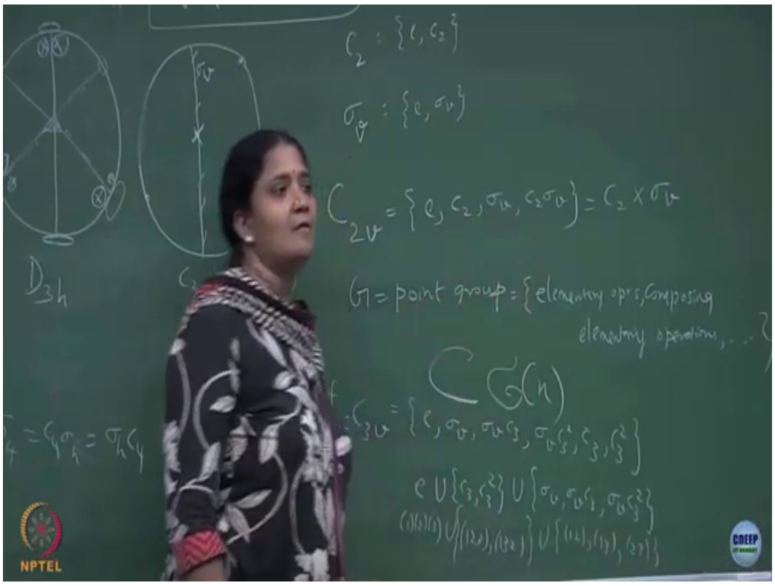

And clearly once I have written this the properties which you have if you multiply sigma v with sorry the sigma v with C 2 you will get one of those elements which is C 2 sigma v and you can verify that. Those are the other two mirror planes which you have. One mirror plane was sigma v, C 2 sigma v is the other mirror plane. So, you get the other mirror plane ok.

So, how many classes are there here? How many conjugacy classes are there in C 2v? It is an Abelian group. It is a class every element is a class by itself right. Once it is an Abelian group similarity transformation does nothing. So, there will be the order of the group itself will be the class. So, let us write for C 3 the matrix representation. This is something which you all know how to write.

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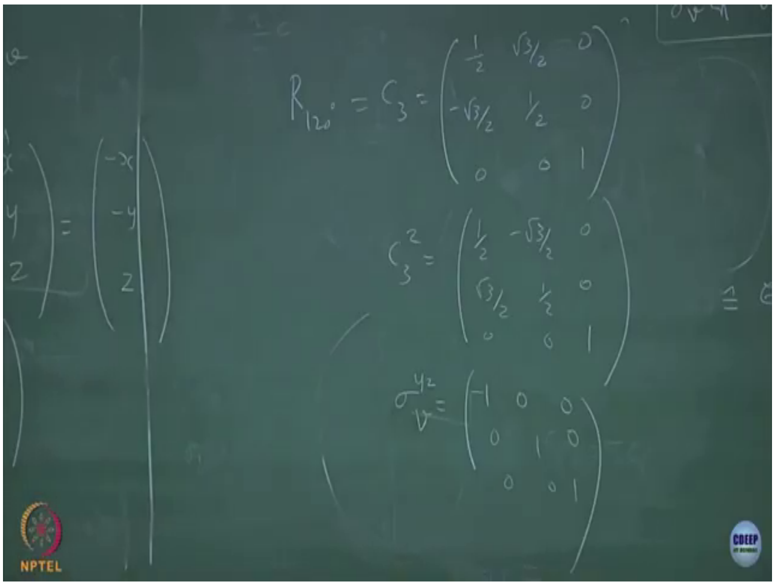

R 120 degrees which is what we call it as C 3 matrix will be cos 120 which is sin 30, is that right? And, C 3 squared is right and then let us write sigma v also S 2 C 3 sigma v C 3v. Sigma v will be let us take it to be in the y z plane, then you are all with me?

Now, you can generate other elements of the C 3v group. How do you do it? You just multiply things. You multiply this with this C 3 squared with this right. We can start generating the other two elements right. Once you have a sigma v you start multiplying in C how many non trivial elements you get and you generate a representation a matrix representation for the C 3v group. After we have got the representation we would like to see what is the irreducible representation ok, that is the next topic ok.

So, there will be an irreducible representation, what does irreducible mean? I cannot further break it any more that is what is the meaning of reducible. So, I need to find some set of non-trivial irreducible representations for each of these groups and the thing you have to also realize is if you take the trace of this matrix trace, this is 2 right this one is also 2. These two are conjugate elements; conjugate elements will share the same trace.

So, your representations which you write will also have that property that the trace within a conjugacy class cannot change ok. So, this trace and if you multiply this with sigma v and write that trace should also not changed.