Group Theory Methods in Physics
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Lecture – 11
Point Groups

So, now, that we have introduced concepts of finite group and also, I said that they can all be these finite groups, can all be subgroups of the symmetric group of n objects, where it involves permutations of n objects, which we call it as symmetric group of degree n.

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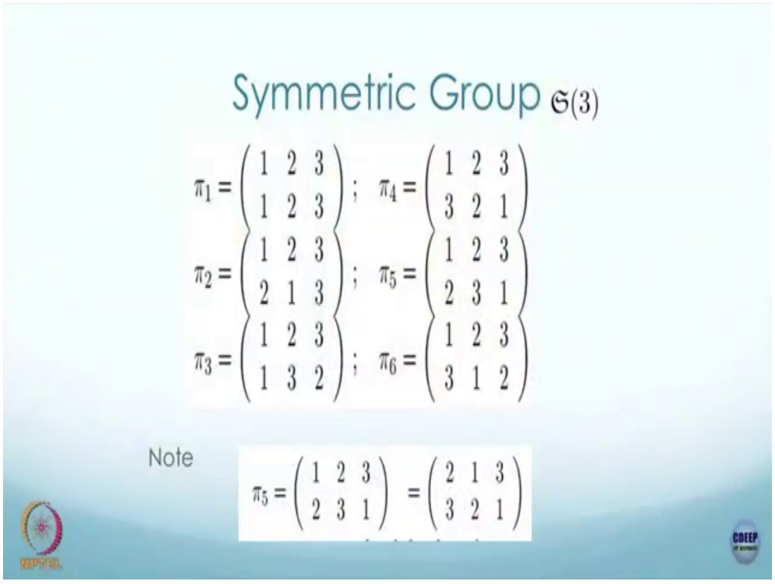

We are now in a position to look at how these applications are looked at in molecules which is composed of atoms and these molecules have certain symmetries. This is what I was trying to say in the last class.

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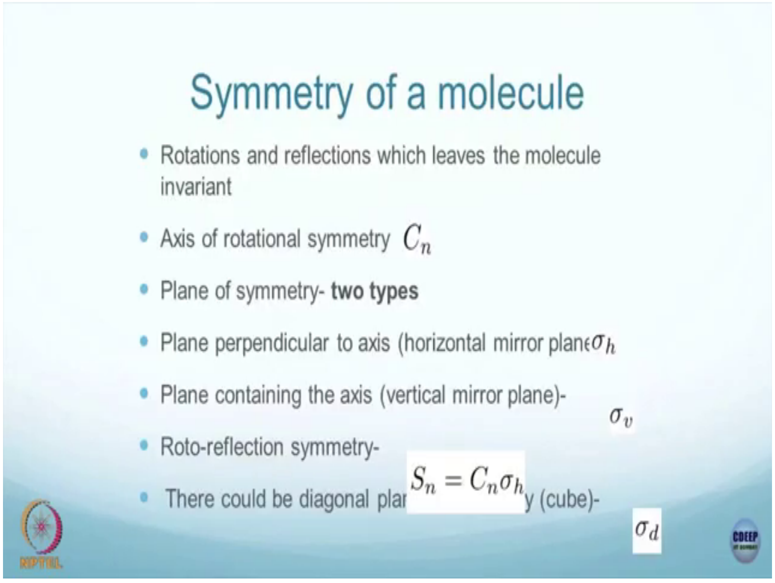

I did start off saying that you can have configurations of atom in a molecule and you will have a symmetry axis; one of them is the conventional rotational axis and depending upon what symmetry you have, if the configuration is such that it has a symmetry where by doing pi by 2 rotation, you get back the same atom. Like one atom goes into the place of the other atom and it looks exactly similar to the earlier configuration, then you will say that it has a fourfold symmetry right. 2 pi by n is the rotation. Is that clear? Everybody is with me?.

So, this is also similar to your cyclic group which we were studying, where you had a generator. Sometimes people use synonymously C n as an element and when they write the set for the C n group, you write identity C n, C n squared and go on till C n to the power of n minus 1.

So, this is it is used as sometimes also as a generator ok. Besides the axis of symmetry, so various rotational 2 pi by n rotations, you could also have planes of symmetry ok. One plane could be containing the symmetry axis n fold symmetry axis, other plane could be perpendicular to the symmetry axis. Some of that notations which I have followed are that sigma h is the plane which is perpendicular to the symmetry axis and sigma v is when it contains the symmetry axis.

Not all molecules will have these symmetries ok. So, that also you should remember. You have to look at the molecule and see what all the possible symmetries are there. If you do a sigma h, if it goes into a configuration where atoms do not go into each other, then it is not a symmetry of that molecule ok. So, you have to see what is the principal axis. So, the main axis of rotation symmetry with the higher value of n is what is called as a principal axis.

So, you have to see what is the principal axis symmetry. We saw this in the last class I showed you a water molecule, I showed you ammonia molecule. You know look looking at it that the rotational axis has to be threefold for ammonia molecule, where the axis has to pass through the nitrogen and similarly, in the hydrogen in the water molecule the axis has to pass through the hydrogen and you have this sorry oxygen so that you have this rotation which is 180 degree rotation right.

So, you can recall pictorially what is happening whatever I have been saying as a group theory tool with elements generator. Now, you can see it as an elementary operation of which you do in this configuration of atom which constitute a molecule. So, this is basically a roto-reflection.

So, sometimes the molecule will not have a pure rotational axis, it will not have a pure mirror plane symmetry, but you could do something like do a rotation and then, a reflection and that combination maybe a symmetry. I will show you a couple of things that you understand it is called roto-reflection.

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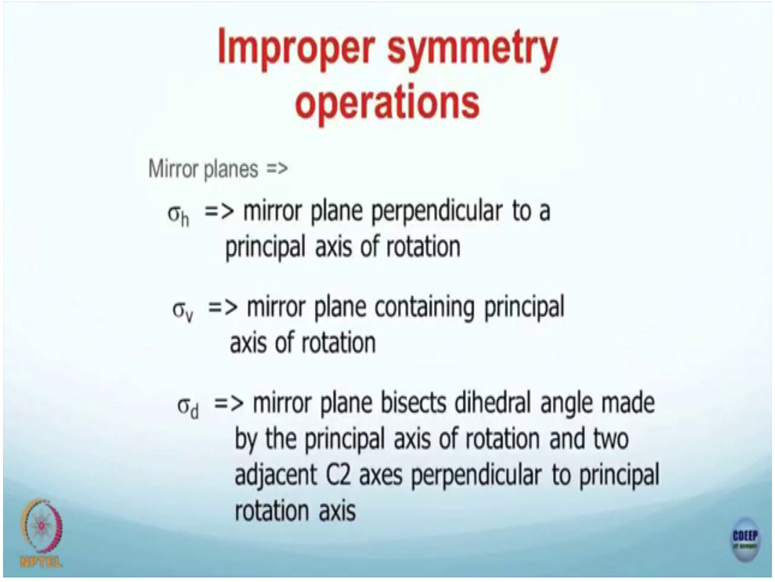

And there could also be diagonal plane. So, let me just go again on this since it is. So, the mirror planes can be of types like one as I said mirror plane could be perpendicular to the principal axis of rotation ok. And then, there could be another mirror plane, where you have the mirror plane being containing the axis of rotation. So, the principal axis means a one whose rotation angle 2 pi by n, the n fold axis n which is the maximum is what we call it as the principal axis.

Sometimes you know you look at a molecule, it will have a twofold axis symmetry, it will have a threefold axis symmetry, it will have a fourfold axis symmetry. If you have that, then the principal axis is only the fourfold axis ok. So, the others are all not the principal axis in it and if the sigma v plane which you are going to consider contains that principal axis, then you call it to be the notation is sigma subscript v and that is a plane of symmetry.

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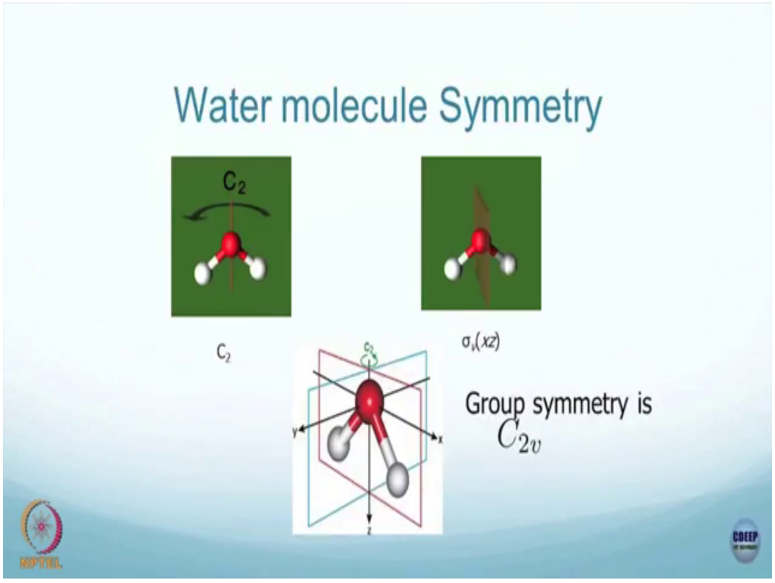

For example, in these examples which I talked the principal axis is only the twofold axis rotation by 2 pi by 2 ok.

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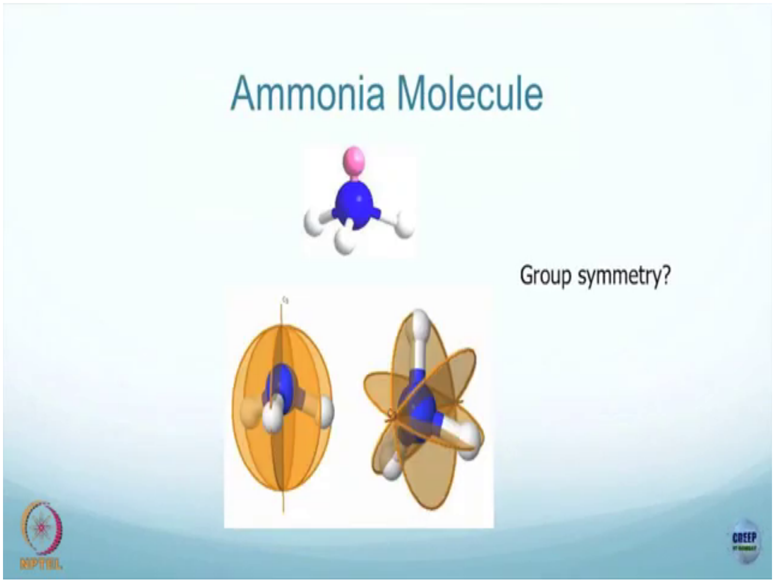

If you look at this ammonia molecule, you can see that the principal axis is a 2 pi by 3 rotation ok.

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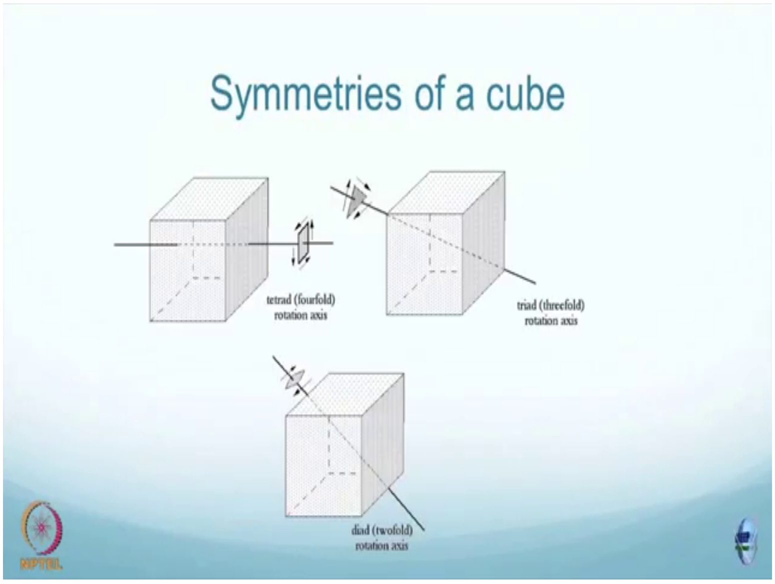

So, here you have only one axis. So, it is not very, you do not need to worry so much about principal axis, but if you see the cube ok; the cube has fourfold axis rotation. How many of them are there? There will be 3 of them right. Along this axis, if you do a rotation about this axis, the cube remains the configuration remains the same; but there can be 3 axis right, one this way and then the other face right.

There could also be a threefold rotation axis. So, in this case you will say the principal axis is of fourfold axis. If suppose, the atoms are placed on a cube which constitutes a molecule which has this cubic symmetry, then the principal axis of rotational symmetry for the molecule which has this cubic symmetry is fourfold axis, it is a notation. So, typically when we look at molecules, we start looking at what are the basic axis of symmetry, planes of symmetry for the molecule. Those are the elementary operations.

It is exactly like generators of your group which we will study and then, you start composing all possibilities of these axis of symmetry and planes of symmetry and you start generating the finite set and their formal group ok. So, this is the group which is group symmetry associated with the molecule, which is constituting that configuration of atoms. For example, ammonia molecule ok. These notations as I said already these notations are important only when you have a principal axis of symmetry, otherwise you just call it as a mirror plane sigma ok.

So, there are these additional mirror planes which is called diagonal mirror planes, if you have this dihedral group I said, but then we will see how to see the dihedral group in the molecular language in the molecular structure language and in those cases you can start seeing if there is a diagonals by section which you find and then you start talking about diagonal mirror. So, we will see one or few examples so, that you start understanding this notation ok.

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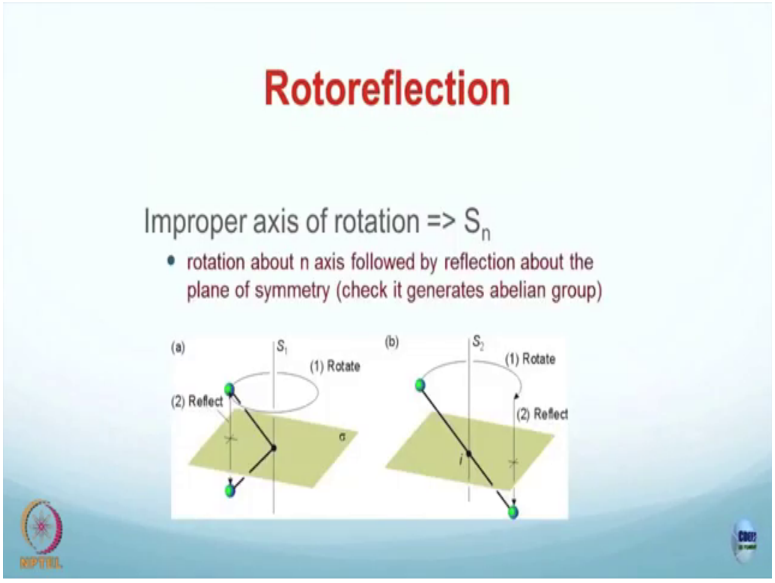

It is just to say a few lines about Rotoreflection. Rotoreflection, the symbol is S subscript n. What it means is that rotate about and nfold axis; that means, you do a 2 pi by n rotation followed by our reflection about the plane of the symmetry ok. So, the plane of the symmetry is perpendicular to the axis of rotation. What does that plane called? Sigma h ok.

Sigma h if it is this is the axis of rotation, the plane is perpendicular to the axis of rotation, we call that plane to be a sigma h plane. Subscript 1 means you do no rotation right; you do not do rotation at all. So, you have an element, rotation about n fold axis is identity operation and then, you do a reflection about the plane which means if this element goes here below.

Are you all with me? This is what is roto reflection S 1 it is nothing but it is just the mirror symmetry right. S 1 is isomorphic to sigma h and sigma h is made of element identity and the mirror transformation ok.

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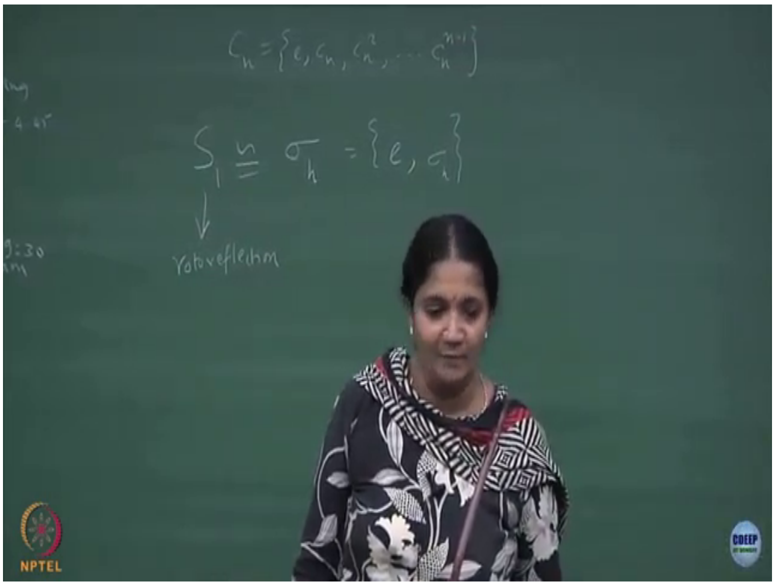

S 1 is what? It is a roto reflection, roto reflection and this 1 denotes rotation by 2 pi by 1 which is 2 pi rotation and then, you do a reflection on a plane which is perpendicular to the axis. Is that clear? And S 1 is nothing but your just the mirror plane symmetry and that also forms a order to trivial group. As I said generators are sometimes written as the group element also. The group is also denoted by the generator ok. Like for example, C n you can write it as e C n, C n squared ok.

This is the way of writing. So, let us look at S 2. What happens to S 2? S 2 you have to do a rotation by 2 pi by 2 which is 180-degree rotation right. You take this atom do a 180-degree rotation, but that is not roto reflection. You have to do a reflection about this plane and you get this point ok. So, is that right? Is it clear to you from that picture? So, this is nothing but your inversion group given an atom, you have a by an inversion.

Suppose you have a vector, let us take a sphere. If you take a point here, the point completely diametrically opposite to it can be seen as an inversion about the centre right. You can see it as an inversion about the center. This is exactly what is happening this S 2 is a roto reflection with rotation by 180 degrees and then a reflection that symmetry group is isomorphic to an inversion group which is denoted as C subscript i. Do not confuse this i with n. This is made of identity and an inversion.I squad is also e, but i is an inversion.

So, given a vector r and their inversion, you go to minus r, that is what is the inversion. Clear? So, the roto reflection symmetries are seen in some atoms and you have to remember that this is the this is also a 2 element group. S 2 is not isomorphic to C 2. So, you have S 2 which involves inversion C 2 which involves pure rotations ok. So, then there are a lot of distinctions which you have to see from these groups ok.

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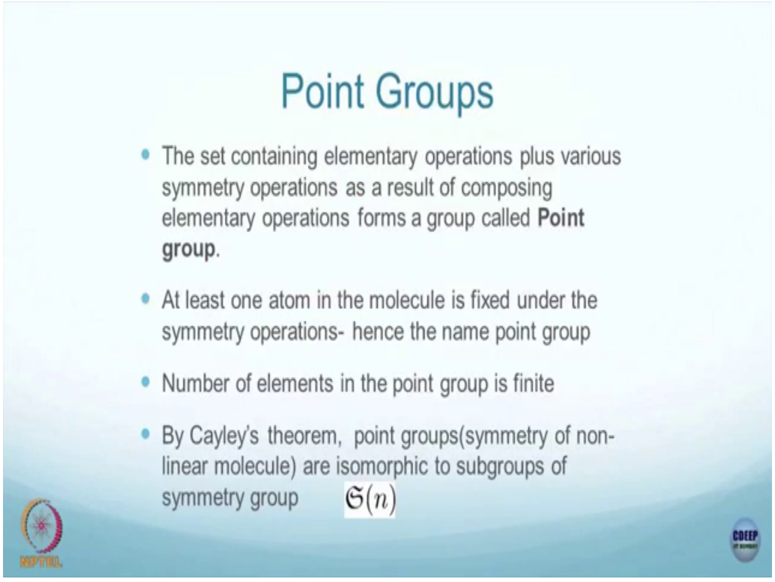

So, now that I have given you some flavor of how the atoms can be distributed in a molecule, which has some kind of a symmetry structure which we can call it as a molecular symmetry. We will start looking at from the group theory point of view what we studied earlier. The set of set containing elementary operations; elementary operations could be rotation about principal axis, it could be reflection about the planes of symmetry ok.

So, those are elementary operation and then, you can also compose these elementary operations. You can do a rotation and then, a reflection if reflection is also symmetry of the system. So, you start writing that set ok. So, that is what I did for the water molecule right. So, when it took the water molecule, I saw it has a C 2 symmetry, I saw it had a sigma v symmetry. C 2 is nothing but identity and C 2; sigma v is nothing but identity and sigma v. These are the elementary operations.

You can compose these elementary operations and write a set which you call it a C 2 v which is e C 2 sigma v C 2 sigma and it is nothing but a direct product of it is a direct product group for an example ok.

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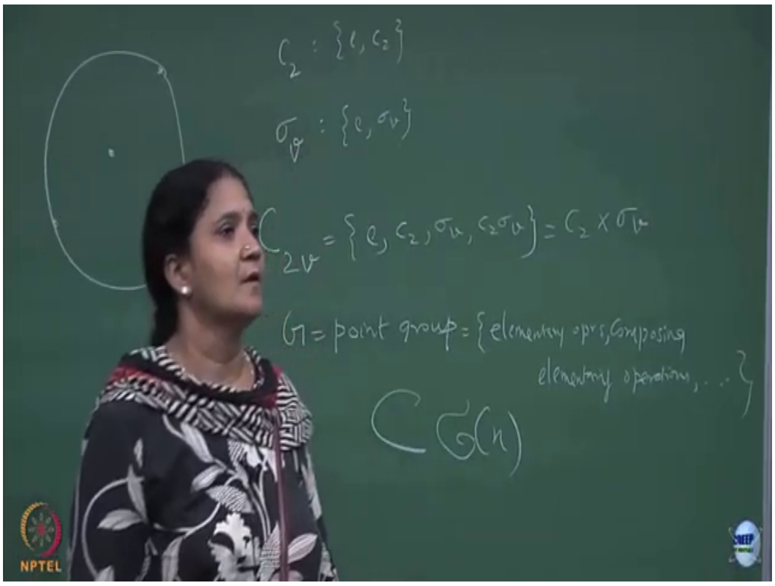

So, this set which you are constructing is a finite group and this finite group which you this is for example a molecule I took the water molecule, but you can write for many molecules, different group symmetries. And this we call it as a Point group; in the context of molecules, we call this is a point group which is made up of elementary operations and then, composing elementary operations and it is that said should satisfy those properties of the 4 axioms of the group ok. And each of these group with you are going to find, we will always be a subset of some symmetry group. What does that theorem?

Student: Kaylee’s theorem.

Kaylee’s theorem. So, all these point groups which, why is it called point group? Anybody, can know why the name point group came in the context of molecular symmetries? At least one point in the molecule through which the principle axis goes right? Take an ammonia molecule, nitrogen atom is not moved by any of the transformations ok. Similarly, the oxygen atom is not moved by the C 2 or C. At least, 1 atom will remain untouched, that is why they got this name point group. At least one point in the configuration of an atom is going to be remaining fixed under all the elements of the group ok.

Student: Maam, if we take a cube and (Refer Time: 17:43) corners, then we rotate that?

Correct.

Student: Again, all the (Refer Time: 17:48).

Good. So, for the cube and other symmetries are a little more than the point group symmetries which I am looking at it. So, there if you think there is a atom at the center of the cube, then you can think that point is not and untouched. So, it is if you look at it as a methane molecule like for example, if you take a methane molecule, if you put the axis through the carbon, that carbon remains invariant.

So, in the context of these molecular. So, cube was just a simple example to show you that you know you can look at it this way. But in general, there will be always a point which I would not I do not need to touch by any of these transformations. The center point of the cube will not be touched. Whether there is an atom at the centre point is your question, but I could have put an atom there and still the cubic symmetry will be still there right. So, that is what I mean with this.

Student: Maam, on a (Refer Time: 18:53) reflection group, is it fair to say that we can (Refer Time: 18:59) right, we can map it to some other rotative rotation.

That is a good point. See first of all pure rotations are completely different from reflections, you know why right. If you take a plane and do a rotation, the determinant of these matrices when you write it, you can never make it negative right? But when you do a reflection, the determinant can become negative, you can never transform pure rotations to become improper transformations.

So, roto reflection can never be made into look like a C n. If at all you want to make a roto reflection to look at some other point group, it should have an improper transformation component in it.

Student: Can you find the plane where it is purely a reflection?

Purely a?

Student: Reflection.

S 1 for example, is a purely a reflection; roto reflection S 1.

Student: But it is generally true.

It is not generally true. It will have, it will we will see some more examples and then you can, I will give more problems and then we can see all those ok. So, but as of now you should distinguish the pure rotation which is about an axis of rotation is very different from the reflection planes, inversion symmetry point ok. They are all improper transformations. Is that clear? You never make a composition of rotations to look like a reflection, that is all I am trying to say.

Whatever composition of rotations you take, it will never give you. It is clear know, if you do C 2 and then a C 2 square, you are not going to get sigma v at all. Sigma v is a distinct generator and these two composed one will be this this element you can call it to be an improper transformation. Because C 2 is a proper transformation or proper rotation; sigma v is a reflection. Combining a reflection with a proper rotation is an improper transformation ok.

So, the number of elements in a point group, I have kind of given you a flavor with some examples like ammonia molecule and water molecule that you do see that the number of elements which we write by looking at the symmetry of a molecule, I can construct this and the number of elements will be finite and there will be subgroups of symmetric group of degree n.