Chemical Applications of Symmetry and Group Theory
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Lecture – 02

Hello, good morning. So, today is the second day of this course. So, in the last class, if you remember, we talked about the symmetry aspects of different objects and different molecules, I showed you quite a number of structures of different objects as well as certain molecules. And we discussed about the symmetry aspects of those. And we say that ok some molecules are most symmetric than others; and ultimately we also showed that there is something called symmetry element and symmetry operation, which is like symmetry operation is the movement of a body by which end up having an indistinguishable structures. And today what we are going to do we want to find out about the symmetry elements and symmetry operations in bit more detail.

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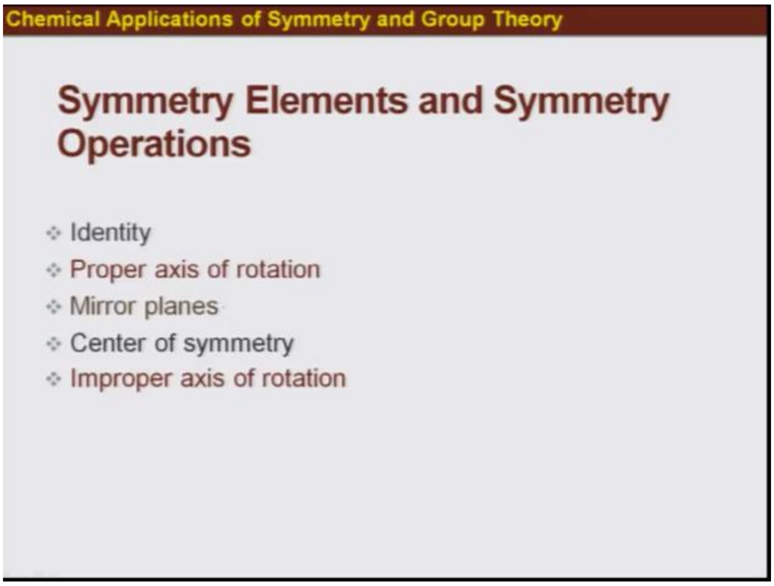

So, what are the symmetry elements and symmetry operations that a molecule can have? So, one can have five different symmetry elements, and we can generate several symmetry operations out of those elements. We will look at that in greater detail. So, let us look at one-by-one. So, as you can see on the screen that you can have an element called identity, another element called proper axis of rotation, and you can have mirror planes, you can have center of symmetry, and you can have improper axis of rotation. So, now, let us look at one-by-one what is what.

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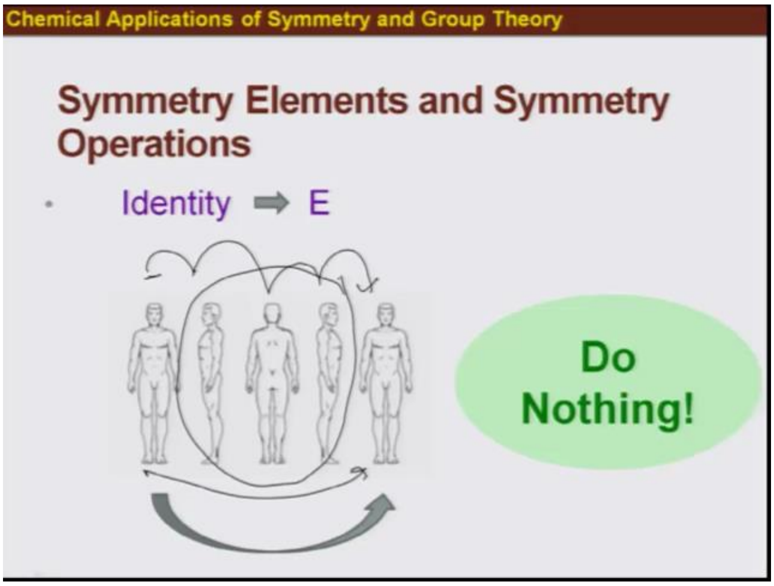

First let us look at identity you know the element of identity. So, what is it? So, before going to the details of this identity operation and all these things let us also see what this identity of operation is denoted as, identity operation this is denoted as E. Now, what is this identity operation? Before going into the molecular structure, I will give you very simple you know representation of this identity operation. Suppose, a person is looking at a particular direction then he can take several turns. So, one can take a complete right turn that is by 90 degree. So, if I take a right turn, I will be looking at this direction. And then if I take another right turn then I will look at the back that is towards the board, and then two more right turns I will come here.

So, there is very nice stories about you know United States Army drills, so in army drill what we have is a commander will tell you to take a particular position they call it take a face. So, what commander will take right face, left face? So, you move by you know rotate by in 90 degree either on the right side or left side. So, there is another turn that is by 180 degree you actually taken an about turn, this is called an about turn. Now, the commander says take an about turn and then he takes one more about turn.

Now, sometime in the drill, the veterans the aged person who has retired from army, they come and take part in the drill. So, one of the veteran, he was taken part in the drill, and then when he heard the about turn command, he starts turning around by 180 degree. While taking this turn, he realizes that he is old enough and is very difficult for him to take turn a proper way he twisting his leg and all these things. And he knew that the in a commander will ask him to turn around again. So, he as to take two about turns, so he realizes that well ultimately I will be looking at the commander at the end after taking two about turns. So, if I do nothing then also I am having the same position. So, this idea of do nothing is actually an identity operation.

So, if you look at this picture here, the person is looking at us, and then he takes keeps on taking turns from here to here and then here to here and then here to here and then here. So, ultimately there is no change in the position of the person. So, now, if I do not go through all these intermediate steps, and if I come from this state to this state directly, the symmetry operation that we have performed is an identity operation. So, essentially you can figure out identity operation means you do nothing, you keep an object as such in his position you get obviously, the identical structure because you are not done anything. So, this identity operation is also called do nothing operation. And this is the easiest thing and no matter what any objects in this universe will have at least one symmetry element in it and that is this identity element. So, anyone can do an identity operation on any object and get an identical structure. Here is identical not only indistinguishable, so that is about identical operation E.

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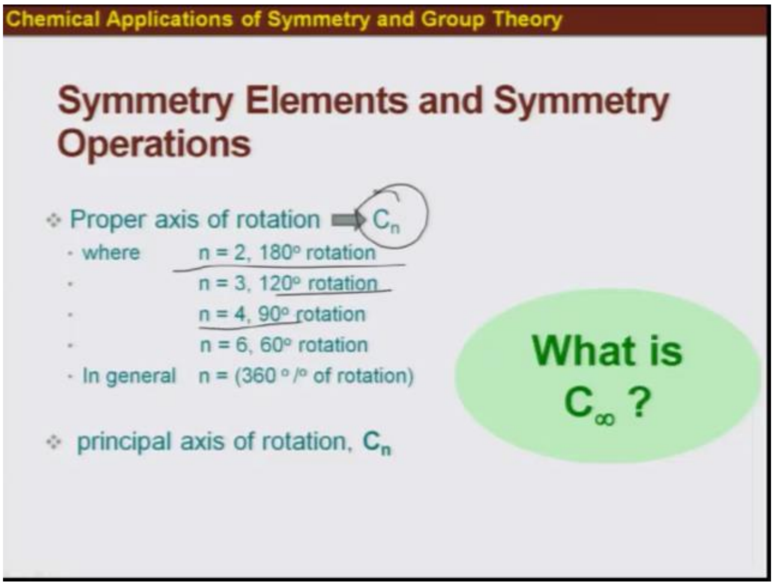

Next, we talk about rotational symmetry elements. This is also called proper axis of rotation. Why this is called proper, we will talk about this in during this course. But less for the being just call it as a proper axis of rotation. So, in the last class, I showed you an example of rotating at equilateral triangle by 120 degree and getting back in distinguishable structures, so that particular axis is called axis of proper rotation. And this axis of proper rotation, this symmetry element is designated by this C n, C subscript n. Now, in that particular example that I give you in the last class we had a 120 degree rotation about that particular axis which is perpendicular to that triangle.

So, what is this n? So, you can see that for C n, n is equals to 2, we have a 180 degree rotation. If I have a 120 degree rotation, and we can get an in distinguishable object, then the order of this rotation, this n here that is written in this C n is called order of rotation. So, for a 120 degree rotation, you have an order because to 3. Similarly, for a 90 degree rotation you can have an order four. So, you can easily figure out that.

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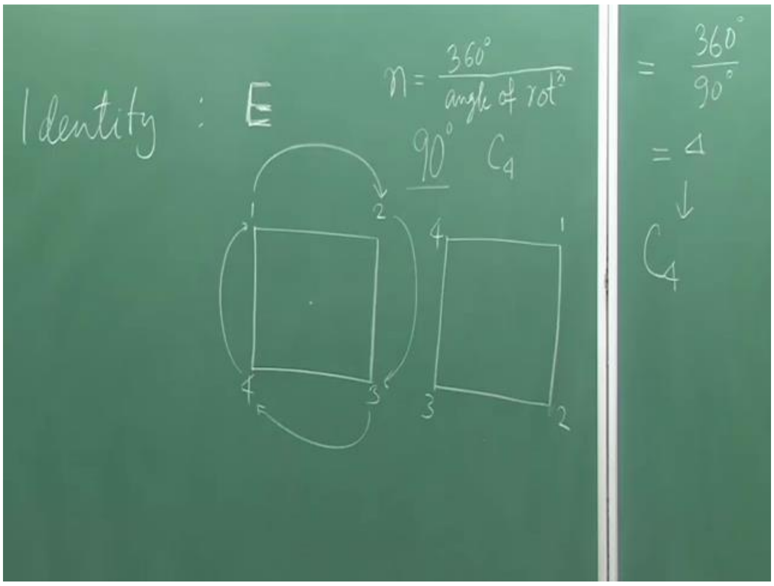

If you have say objects like a square a perfect square. You can imagine an axis through this point, and this axis is perpendicular this plane of the board then for every 90 degree rotation you get an indistinguishable structure. Because this if I mark 1, 2, 3, 4, now we can easily do because you have already seen it for the triangular case, you have another square because square is not going to be changes to a triangle right square will remain a square. So, when you give a 90-degree rotation, so one will come here, two will go here, three will go here and four will go here. So, ultimately what you have is this 1, 2, 3, 4 until and unless you have this numbers you have an indistinguishable structure that is a square. And this is done by a rotation by 90 degree.

So, this axis this C n here is known as C 4 and 4 comes from this relation, where your n is equals to 360-degree by the angle of rotation. So, here it is this rotation is about 90 degree. So, the angle will be 360-degrees by 90-degree is equal to 4. So, I have an axis C 4. So, in that way if I have a rotation of 60degrees, 30 degrees, I can find out what is the order of rotation and the name of the particular rotational symmetry that is C 10, C 8, C 6, whatever. For a 60 degrees rotation, for example, it will be C 6 because 360 degree by 50 degree right, so it will be C 6. Now, you can see that you are I can vary the value of n, I can go from say like C 3 4, 5, 6.

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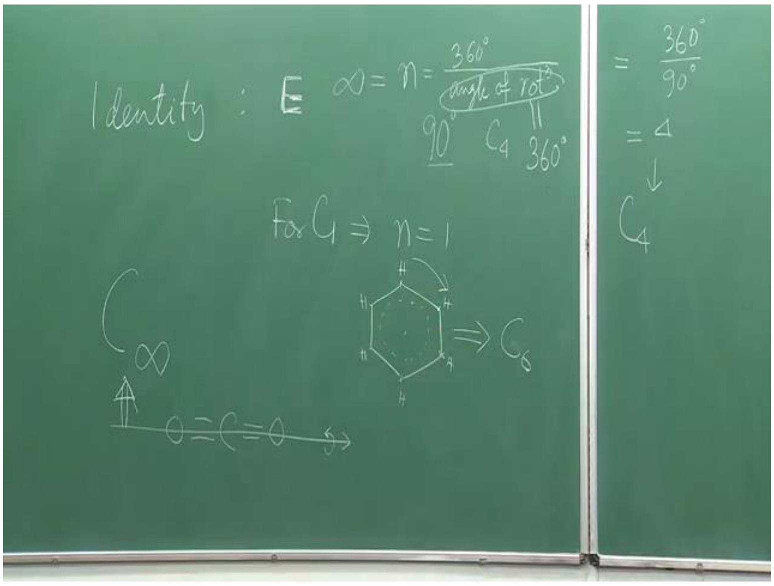

So, I have not written there C 1 why not because C 1 will mean what C 1 will mean from this particular relation it will mean that, for C 1 n equals to 1. So, n is equals to 1 means I must have a situation why this angle of rotation this equals to 360 degrees this is exactly the case what we described just sometimes back when you are discussing about the identity operation, so that is why C 1 is not mentioned anywhere because C 1 and E are the same. So, we have seen that n can be like 2, 3, 4, 5, 6, 7, 8 depending on the structure of the object or structure of the molecule in particular. So, like for benzene I have, so C 6. So, benzene structure is like this. So, this position of the carbon atoms and associated hydrazine's and if assume equal distribution of by cloud then I can have an equivalent or indistinguishable structure for every 60 degree rotation about the axis which passes through this one. So, every 60 degree, I can have the indistinguishable structure and we can have for this one and axis C 6 and this particular is axis is C 6.

Now, in that way, I can go increasing, increasing, and so can I have something, which is c infinity that is a question? So, from this expression, it looks like yes I can have. What is the solution that means; here I have to have n equals to infinity. So, if I equate this one to be infinity what do I have here, I have extremely large number right almost like an infinity. So, in that case, what I have, I have a situation like an object or a molecule which has an axis about which I can give any turn by any amount of angle and I can get an indistinguishable structure.

You need an example. So, here is one example for you carbon dioxide. Now, look at the axis. If I have an axis passing through all these atoms, this is the linear molecule carbon dioxide is a linear molecule. And if have an axis passing through this linear molecule through all the atoms then you see about this axis all around, this is highly symmetric. So, does not matter whatever be the angle by which I rotate it gives an indistinguishable structure. So, in a sense, I can give an infinite amount of rotation before it comes back to its original configuration correct. So, because I can give this infinite degree of rotation about this axis and get indistinguishable structure, this axis is known as C infinity.

Now, we say that this operation is called rotation and really you should say it is a proper rotation. Why it is proper, because if I really can have axis that will change this molecular configuration from one to another indistinguishable one. So, there can be really an axis there, so that means, there will be something which is not like this that is not a proper rather improper we will come to that it is there and we will come to that.

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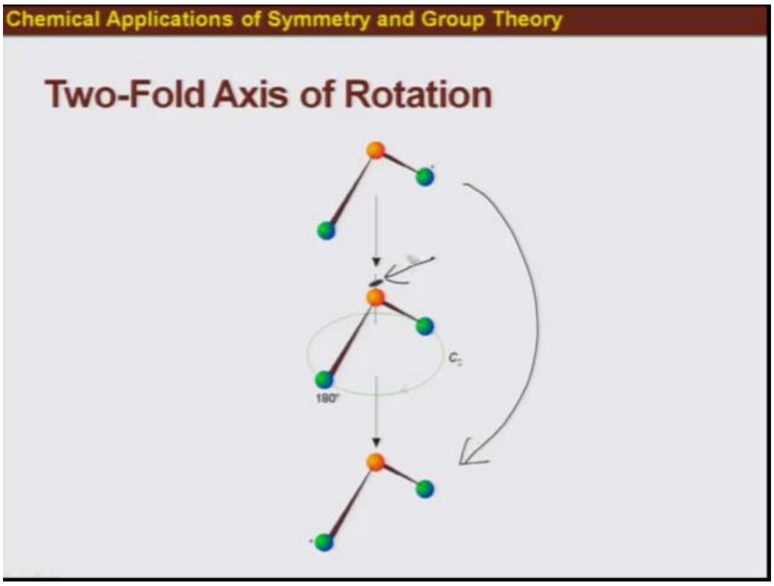

Now, let us see some more example of this rotation. So, as I said that we can have C 2, C 3, C 4 and so on. So, here is an example which shows you the twofold rotation, and the axis about which this twofold rotation is you know taken place is called twofold axis of rotation. So, here we have a molecule H 2 O. So, if I have an axis which bisects the angle H O H then we can rotate the molecule about that axis, it is given here. So, this is that axis about which you can turn them. So, you see we get an indistinguishable structure by a rotation of 120 degree and another rotation by the 120 degree will end of having the same structure back. So, this is an example of C 2.

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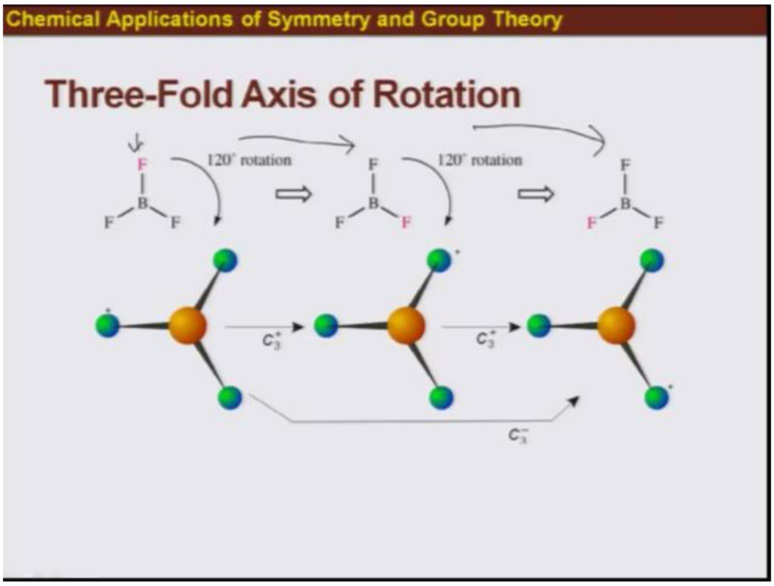

Now, let us come to threefold axis of rotation, which we have already looked at in terms of ammonia. This is another example, which is boron trifluoride. So, here you can see that one fluorine is mutt by a different color then other fluorine, so that you can actually distinguish them. So, now, by 120 degree rotation, you get an indistinguishable structure, but you can actually distinguish still because you have colored one of them separately, but you know its chemistry is not going to change because B F 3 there. So, you can give more rotation and you can change the positions of the fluorine atoms, but they remain indistinguishable though because of the color you can distinguish them here at least on the pen and paper. Now, we have been talking about only one particular axis will about which I can have a proper axis of rotation.

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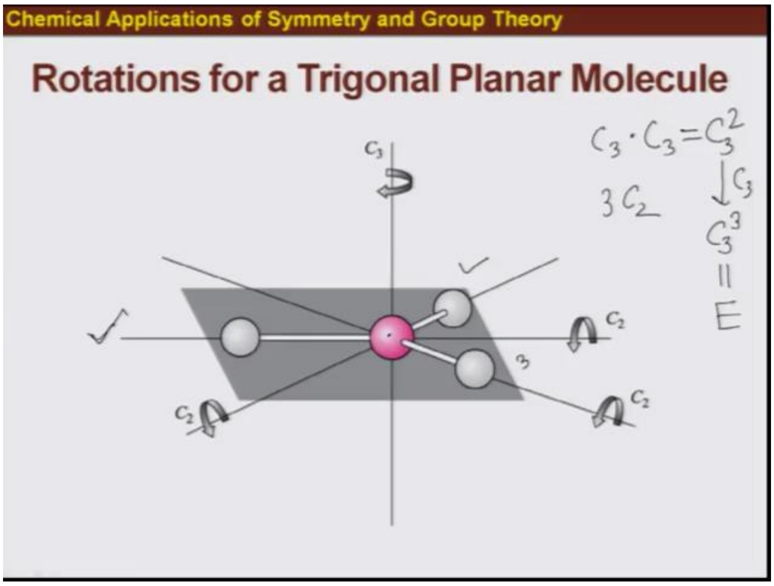

Now, it is not necessary that in a particular molecule we have only one type of axis of rotation. So, here is one example while we talk about trigonal planar molecule. So, say this is boron trifluoride. So, all the atoms are in the same plane. So, it is a trigonal planar. Now, in the last page, we have seen that there is a C 3 axis about which you can have 120 degrees rotation and you can get the identical structure. But is that all, no here you see that I can imagine and axis which right here, which passes through one fluorine and one boron that particular axis you can have an 120 degree rotation about that particular axis, so you can get an indistinguishable structure. So, you have three boron fluoride bonds. So, this is one and this is two and this is three. So, you can have the same type of axis same type of C 2 axis through each of this boron fluoride bonds. So, you can essentially have 3 C 2 axis for this molecule and you can have 1 C 3 axis.

Now, we will also see that this C 3 is an element. Now, when you operate this C 3 consecutively you can get indistinguishable structures. So, you can have C 3 followed by another C 3 and then another C 3 and you can keep going until unless you get an identical structure. So, if you do two successive C 3s then you have something called C 3 square. We will talk about these things much later. And similarly you add one more C 3 into this and you can have C 3 3 which again is nothing but the identity operation, we have already discus that.

So, in this particular case, what we learnt is that a molecule may have more than one type of proper axis of rotation, and here particularly we see that if the molecule as C 3 as well as C 2. And it is also you know not necessary that this C 3 and C 2 that is two different axis of symmetry, they will be coinciding. So, they can have they can be at different plane and different directions or you can have two different axis in the same you know coinciding together.

So, before going to the next one, let me also clarify the last point that I made that is in the case of BF 3 we saw that C 3 and C 2 they are not coinciding, but inside an molecules you can have you know more than one proper axis of symmetry coinciding together. So, for example, you can have let us take this particular molecule Benzene here. So, you have seen that there is an axis about which we can give a 60 degree rotation. And you can have a C 6 axis. Now, for every C 6 turn this hydrogen goes here this hydrogen goes here. So, you give a 60 degree movement here. Now, if you want you can have an axis here and you can rotate in such a way this h comes here that is I can have 180-degree rotation, so this 180-degree rotation about this axis without going through this. So, directly you rotate and bring it here, do not stop here. So, this is a C 2 axis. So, C 2 and C 6, they are about the same axis, so which is different from B 3, but again here this is not all, you can have many other rotational axis.

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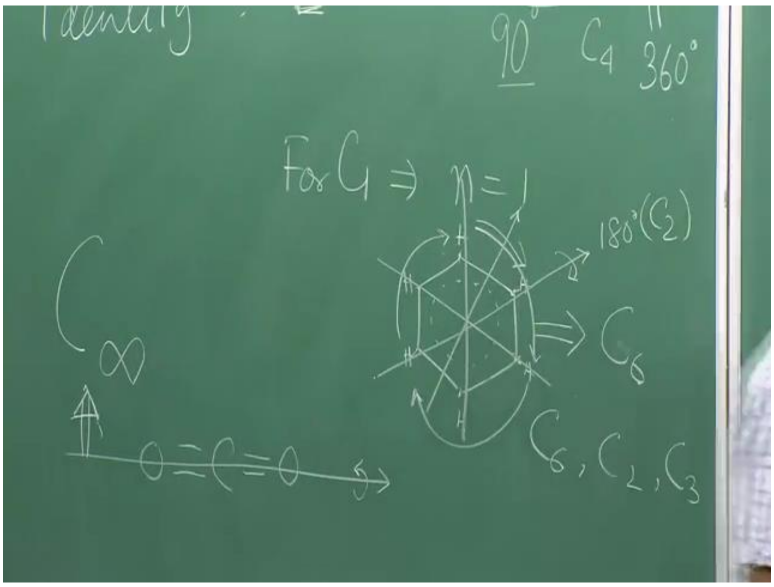

For example, what we can see here that is about this, you have C 6 axis you have C 2 axis. And you can come from here to here directly, and then from here to here, and here to here by 120 degree rotation. So, thereby you have C 3 axis. So, all this C 6, C 2, C 3 they you know coincide on each other; they are about the same physical axis if you can imagine one here. But there is other axis like if you connect this hydrogen to this hydrogen, you find a symmetry axis here about which if you give a rotation of 180-degrees, you will find identical structure because this will come here and this will go here. So, it is just a flipping. So, similarly, this will do the same job, this will also do the same job. And if I can imagine an axis like this, this will also do the same job. So, I can have six different C 2 axis which are lying on the plane of the molecule not coinciding with this C 6 or C 3 or C 2 and this C 2 is different than the C 2 that I just showed you.

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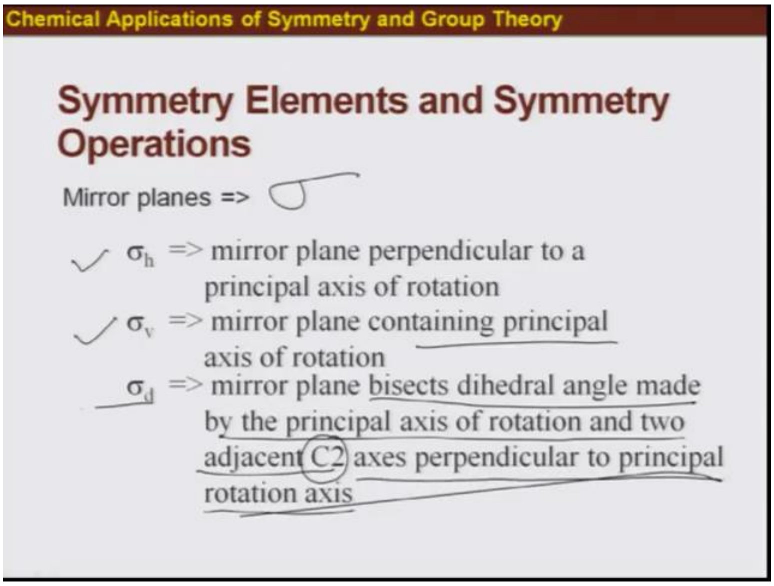

Now, let us move onto the next symmetry element, which is known as a plane of symmetry. So, what is this plane of symmetry operation? So, you imagine any object or any space if you take this x, y, z coordinate and you reflect it about a plane and if you get an identical structure that is having coordinate minus x, minus y, minus z then you get equivalent and you get rather indistinguishable structure by this reflection. So, you are doing a reflection about a plane, and you are getting indistinguishable structure. And this plane is a asymmetric plane. And this symmetry operation is called plane of symmetry or also sometime called reflection operation.

Now, this reflection operation is or the mirror planes they are denoted by a symbol sigma. So, all the plane of symmetry are denoted by the symbol sigma. Now, there can be a different type of sigma. So, you can see that we have something special called sigma h - sigma subscript h. So, sigma h is a mirror plane, which is perpendicular to the principle axis of rotation. Now, you also have something called sigma v; sigma v is also mirror plane, but this particular mirror plane has particular characteristics which say that this particular mirror plane will contain principle axis of rotation. There is another type of mirror plane, which is known as sigma d. So, sigma d is mirror plane that bisects the dihedral angle made by the principle axis of rotation and two adjacent C 2 axes, here one notice this 2 is actually a subscript. So, this mirror plane bisects a dihedral angle made by the principle axis of a rotation and two adjacent C 2 axis which are perpendicular to the principle rotation axis.

So, you can see that whatever be the name sigma v, sigma d or sigma h, their functions are same. So, this subscripts v, d and h just are used to separate different planes of symmetries, but their jobs are same. So, in the following class, we will talk about more about this mirror planes, and we will sight some examples and go to the other kind of symmetry elements and symmetry operations. So, see you again in the next class

Thank you very much.