Symmetry and Group Theory

Prof. Dr. Jeetender Chugh
Department of Chemistry and Biology
Indian Institute of Science Education Research, Pune

Lecture - 05
Planes and Reflections

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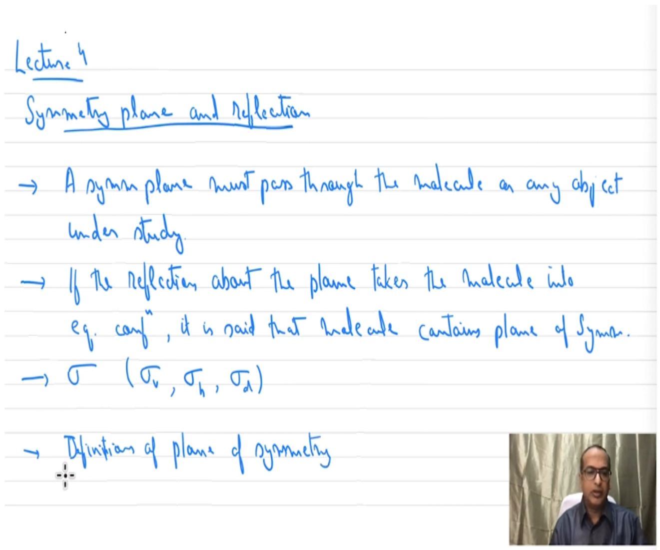

Welcome back everyone, let us start with lecture 4. So, in continuation of our discussion on symmetry elements and symmetry operation, let us today discuss symmetry plane. This is the next symmetry element. Symmetry plane and corresponding operation is reflection. So, before we actually go see examples, let us look at few important points about what symmetry plane is and what is a technical definition etc.

So, first of all a symmetry plane must pass through the molecule. So, it should pass through or cut through the molecule not lie outside the molecule or any object under study. So, if you are studying is something else like not the molecule but any object, so, the symmetry plane must pass through the object under study. So, this point is important because so far we have learned the planes while studying stereochemistry where the planes tend to lie outside the molecule. Also where we are trying to see as super imposable or non-super imposable mirror images.

So, in this case, we do not want to use the same plane. So, here the symmetry plane must pass through the molecule. So, that is why it is this point is made. So, if the reflection about the plane takes the molecule into equivalent configuration, it is said that molecule contains plane of symmetry. Now, the symbol is, we have learned this before, sigma and then there are 3 different types of sigma. Sigma v, sigma h, and sigma d. We will look at the definition of each of this, but let us first look at the technical definition of plane of symmetry. How do we actually carry out the reflection? So, let us see.

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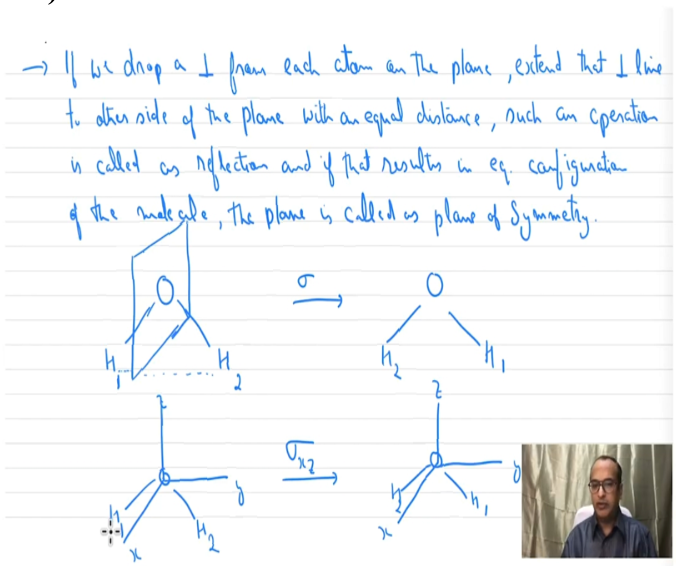

So, if we draw a perpendicular from each atom on the plane of symmetry, then extend that perpendicular line to the other side of the plane with an equal distance of course. Such an operation is called as reflection, and if that results in equivalent configuration of the molecule, the plain is called as plane of symmetry. So, let me read this again. So, if we drop a perpendicular from each atom on the plane, extend that perpendicular line to the other side to the plane with an equal distance. Such an operation is called as reflection and if that results in equivalent configuration of the molecule, the plane is called us plane of symmetry.

So, let us see a plane of symmetry. Let us try to see an example. If we have let us say, a water molecule. And this is my plane of symmetry, which is perpendicular to the plane. If the water molecule is lying in the plane of this board, then plane is perpendicular to the plane of the board. I will also draw it in Cartesian format, if that makes it easier.

So, now I am drawing a perpendicular from this proton, this hydrogen to this plane and then we will take it to opposite direction with equal distance and we should find another hydrogen. So, let us say if this is 1 and this is 2. Reflection about the Sigma will give rise to H2 and H1. So, the 2 hydrogens are swapped between each other. And now because this is an equivalent configuration, this particular plane is called as plane of symmetry, this is what this definition tells you.

So, if it is confusing to see the plane like this, so let us draw it in Cartesian system. x, y, z, oxygen is lying on the origin, the 2 hydrogens are in, which plane, yz plane as we drew earlier and now xz is the plane of symmetry, sigma xz. If I put again 1 and 2, what do we get here? x, y, z, oxygen, hydrogen, hydrogen 2, 1. So, H2 which was earlier lying on the positive side of the yz plane. Now, it goes to the negative side of the yz plane. And similarly, H1 comes back to the positive side. So, this is how plane or the reflection works.

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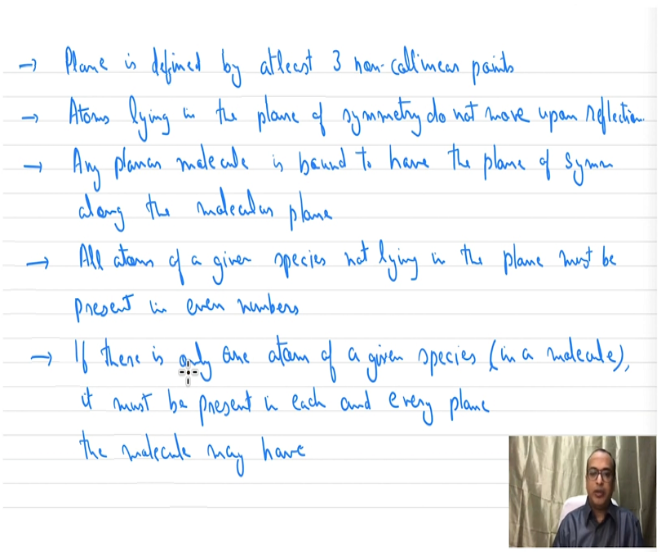

So, let us see few more important points about plane of symmetry. So, we all know plane is defined by at least 3 non collinear points. This is just to give you, you all know this, but this is just to give you again a hint. How do you define the plane?

Atoms lying in the plane of symmetry do not move upon reflection. This we already know because anything which is lying along the symmetry element that atom or point will not will never move or a bond that will never move.

Any planar molecule is bound to have the plane of symmetry along the molecular plane. We will see that again when we look at the examples. So, all atoms of a given species not lying in the plane must be present in even numbers. Again, this will be very clear once you actually look at the examples. So, let me just list down all the properties and then we will look at the examples. So, a corollary from this point - if there is only 1 atom of a given species in a molecule, it must be present in each and every plane the molecule may have.

So, anything which is present as a single number that must be present in each and every plane. This is again obvious. Because if it is not present in each and every plane, you cannot find a partner of that on reflection, and then if you cannot find then there would not be any plane of symmetry present. So, again this will be very clear but when we look at the examples.

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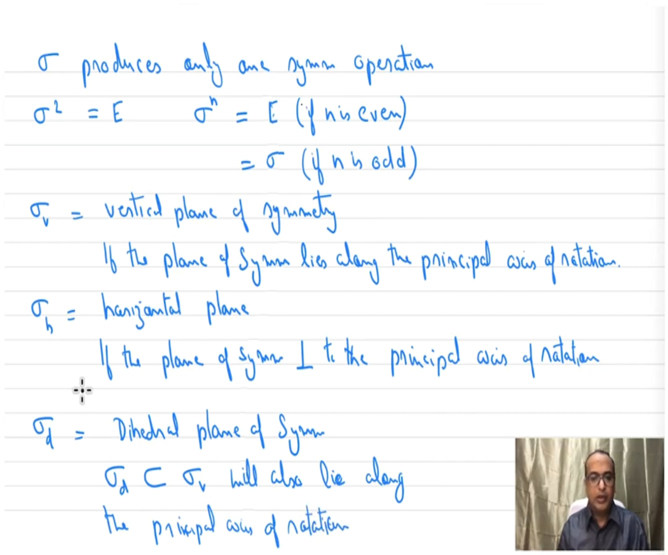

Now, sigma produces only 1 symmetry operation. Unlike proper axis of rotation where we saw that nth order axis will generate n operations. In this case, sigma will produce only 1 symmetry operations. Why it is so? Because if you do 2 sigmas, sigma square, this will be equal to E, because the molecule will go back to identical configuration. So, or in other words, if we have sigma raised to the power n will be equal to E if n is even and will be equal to sigma if n is odd.

So, now defining the other 3 categories, sigma v, which is called as vertical plane of symmetry. So, now this is defined as, if the plane of symmetry lies along the principal axis, so, principal axis of rotation, it is called as vertical plane of symmetry. Sigma h that is the horizontal plane, so, by definition now you can make out if the plane of symmetry is perpendicular to the principal axis of rotation, it is called as horizontal plane of symmetry.

Now, let us look at the most crucial 1. Crucial in the sense it is sometimes difficult to judge which one is sigma d which one is sigma v. Dihedral plane of symmetry. So, sigma d, it is a subset of sigma v. So, all sigma d are also sigma v but not the vice versa. All sigma v are not sigma d. So, that means, sigma d will also lie along the principal axis. But there is one more condition to that.

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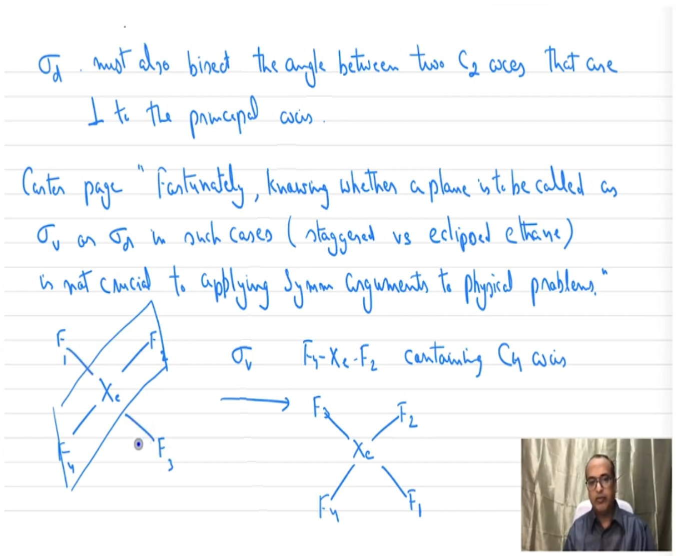

Sigma d must also bisect the angle between 2 C2 axes that are perpendicular to the principal axis. If it fulfils these 2 conditions that it must lie along the principal axis and it must bisect an angle between the 2 C2 axes that are perpendicular to the principal axis, then it is called a sigma d or dihedral plane. However, in certain cases you will see, you will encounter certain cases where it is difficult to judge whether it is a sigma v or sigma d.

In those cases, actually it does not really matter to apply symmetry arguments to solve physical problems. So, I will quote Carter here. If you see Carter page 8, it says I am quoting from Carter directly (18:03). "Fortunately, knowing whether a plane is to be called as sigma v or sigma d. In such cases, when they quoted this, they were discussing staggered versus eclipsed ethane molecule, is not crucial, so you will realize why I am quoting this later, is not crucial to applying symmetry arguments to physical problems."

Now let us look at some examples. So, let us start with Xe F F F F. We have 1 2 3 4. Principal axis is C4 axis. We have already seen that C4 axis, which is going through Xe and perpendicular to the plane of the board. So, it is crucial to identify the principal axis because that defines which is your sigma v, which is your sigma d, which is a sigma h and so on. So, let us first list down the Sigma v. So, sigma v will be a plane which is passing through F4, Xe, F2, these 3 atoms and containing C4 axis. It must contain C4 because it has to contain the principal axis then only it will be called as sigma v. So, basically a plane which is containing C4 axis will be perpendicular to this plane of the board and will be passing through F4, Xe, F2 and a symmetry operation along this plane will be actually reflecting F1 and F3. These 3 atoms would not change their positions. Let us do the Sigma operation. What do we get here? So, we will see, F2 and F4 would not change but F1 will be replaced with F3. Because the plane is like this and this atom will be reflected and this bond will be reflected with each other.

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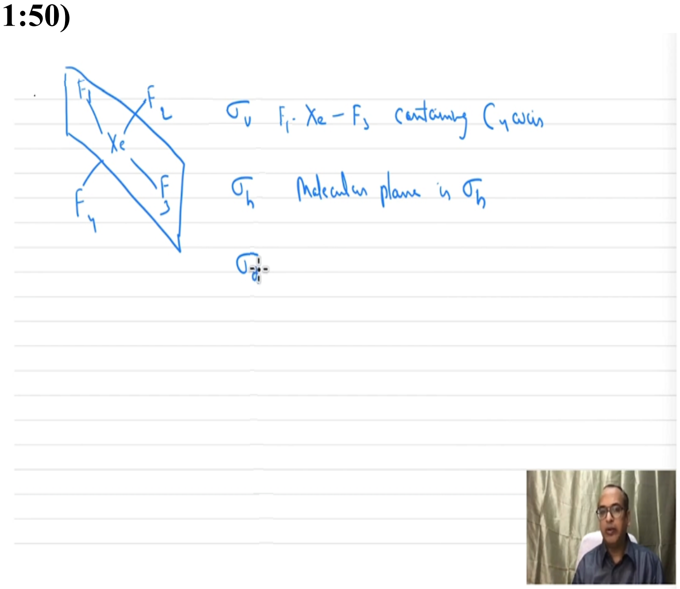

Now, let us go to other plane. So, XeF4, Fs again 1 2 3 4. Other sigma v will be F1 Xe F3. So, I will not do this symmetry operation now, containing C4 axis. It is just to help you identify which plane is this. It is the plane containing these 3 atoms and it is perpendicular to the plane of the board containing C4 axis. Now, let us look at. So, these are the 2 sigma v which are present then there is sigma h because this is a square planar molecule. So, the molecular plane is sigma h and by definition the molecular plane is also perpendicular to C4 axis. It is the principal axis. So, sigma h is the molecular plane. Then we will have sigma d. Now, sigma d has to bisect. It has to contain C4 axis and it has to bisect the angle formed by C2 axis perpendicular to the C4 axis.

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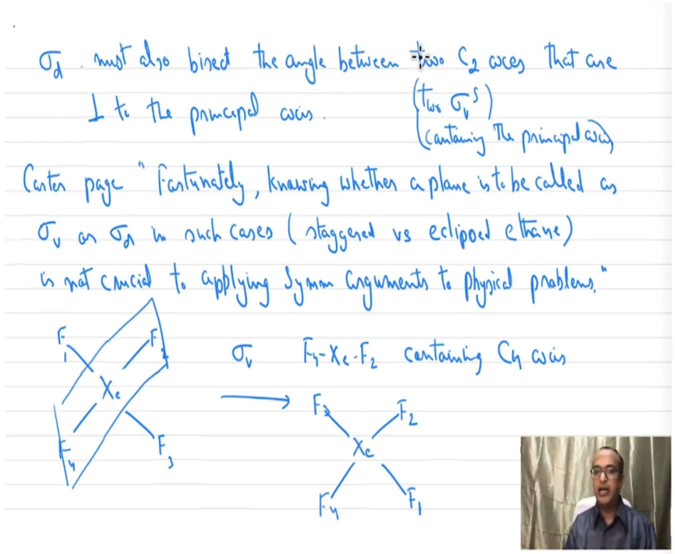

Or in certain cases actually you will see the definition bisect to C2 that are perpendicular to the principal axis. 2 sigma v containing the principal axis. So, it can be either of this. So, if it is bisecting the angle between 2 C2 axis the C2 axis must be perpendicular to the principal axis or if it is bisecting the angle between 2 sigma v. Then sigma v by definition will be containing the principal axis.

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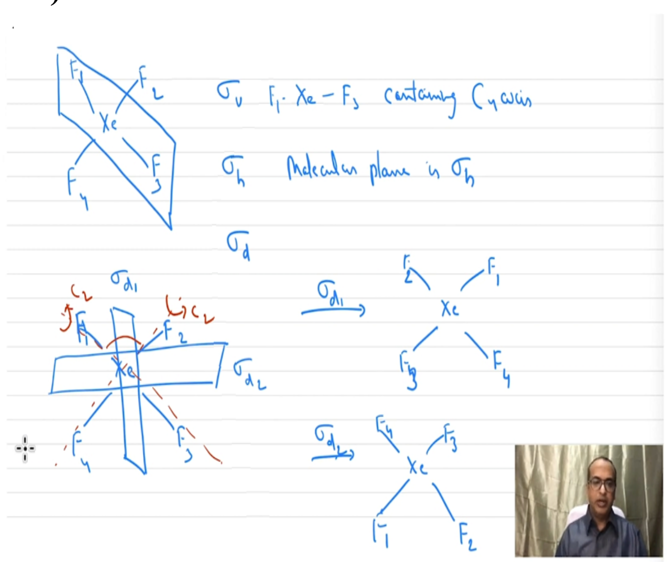

So, let us see this example over here. So, Xe again let me draw this molecule quickly. Now, this particular plane again which is containing this C4 axis. So it is perpendicular to the plane of the board and is actually dissecting the angle, bisecting the angle. This is the C2 axis we have seen earlier. This is the C2 axis we have seen earlier. So, it is bisecting this angle, C2 axis. Similarly, there is another plane which will be dihedral plane which will be like this. So, this is sigma d1. This will be sigma d2.

So, let us also try to do the operations. If we do an operation with sigma d1 and if we do an operation with sigma d2. What do we get? We will get equivalent configuration in both the cases, but what will be the arrangement of atoms. So, if we do sigma d1, F1 will be reflected with F2. So, we will have F2 F1 replaced and F3 F4 replaced. So, this will be F3 and F4. Similarly, if we are doing sigma d2, it will be. If we do sigma d2, F2 and F3 will be replaced. So, F3 F2 and F1 and F4 will be reflected.

So, is that clear? So, we have 2 sigma v, 2 sigma d, and 1 sigma h in this molecule. I took this example because you have all 3 categories of sigma or plane of symmetry in this one.

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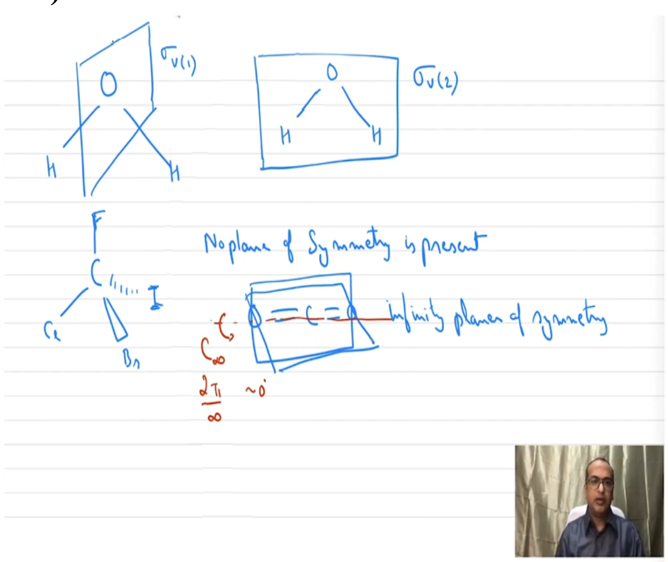

So, now, let us look at again. Let us look at the water molecule where we had seen that earlier. So, one plane was the plane which is reflecting the 2 hydrogens. This is sigma v1, the other plane will be the molecular plane containing all 3 atoms. This will be calling as sigma v2. Now, this will not be called as sigma h because it is not perpendicular to the principal axis. Because both the planes are actually containing the C2 axis here. So, let us also see an example, which is non planar and has all the atoms different.

So, can anyone see that this molecule has a tetrahedral type geometry? But and it does not contain any atom which is repeated. So, in this case there would not be any plane of symmetry. So, no plane of symmetry is present. So, let us also look at the linear molecules. Let us say CO2, how many planes will present? Infinity. So, infinity planes of symmetry as in. so, you have this plane then at slight angle to this. There will be another plane, slight angle to it.

So, it will be all across this axis. So, you have this axis going on. C infinity going through this. So, this is C infinity. So, all of them. So, C infinity is again where the rotation is by 2 pi / infinity. That is rotation is close to 0 degree. Any rotation about this molecule will give rise to equivalent configuration that means, it will have infinity such planes. And this axis will be called as C infinity. So, infinity such operations will be there because you can actually carry out the molecular rotation to 0.1 degree, 0.2 degree, 0.3 degree, and so on.

So, you can be close to any small angle. So, it will give rise to identical or equivalent configuration and this it will be called as infinity. Now, the plane line along this infinity axis will be infinity numbers. So, infinity planes of symmetry.

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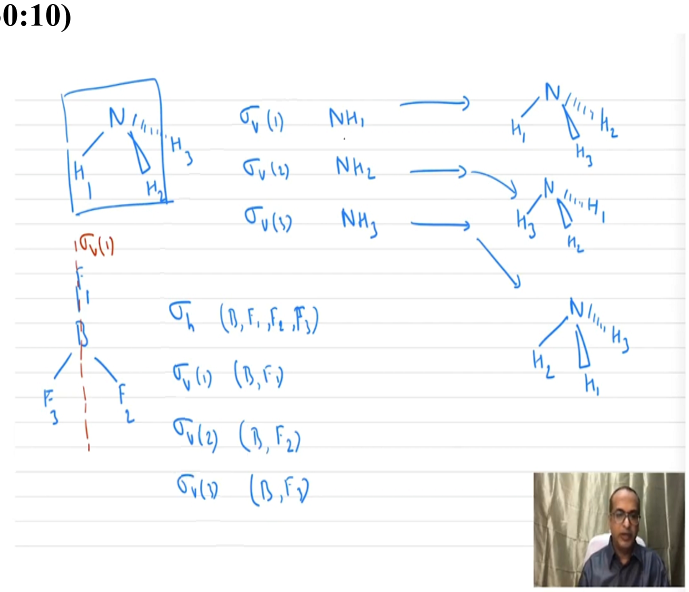

So, let us go forward. Let us look at and NH3 and NH3 is like umbrella like configurations. So, there will be sigma v1 which is passing through NH1, then there will be sigma v2, which is passing through NH2, sigma v3, which is passing through NH3. So, let us see the result in each of the case. So, if we have a sigma v1 which is passing through NH1, it will be reflecting H2 and H3. So, what do we get? NH1 it will not change.

H2 and H3 will be replaced or reflected. So, the plane is like this. So, H 2 is coming out of the plane of the board and H is going behind the plain of the board. So, H2 and H3 will be reflected. H2 and H3 will be reflected while N and H1, they are containing in the plane. So, they will not change. Now, similarly with NH2, if we see now, NH2 will not change. H3 and H1 will be reflected.

So, we will have NH1 and NH3 will be reflected and so on. So, you can think for yourself or this 1. So, NH3 will not be reflected. H2 and H1 will be reflected. So, this should be very simple and straightforward. Now, similarly, look at BF3. We have discussed this molecule earlier where when we were discussing proper axis of rotation. So, if we do. So, we have 1 sigma h which is containing B F 1 F 2 F 3 all 4 atoms basically.

Then we have sigma v1 which is containing B and F1. Then we have sigma v2 which is containing B and F2. Then we have sigma v3 just containing B and F3. So, you should be able to now carry out operations for all these sigma's and see what you get. So, if I just do it 1 quick operation over here. So, let us see. If this is my plain. This will be sigma v1. So, B and F1 would not change. F2 and F3 will be replaced or reflected. Similarly, you can see what will happen if you do sigma h, if you do sigma v2, if you do sigma v3.

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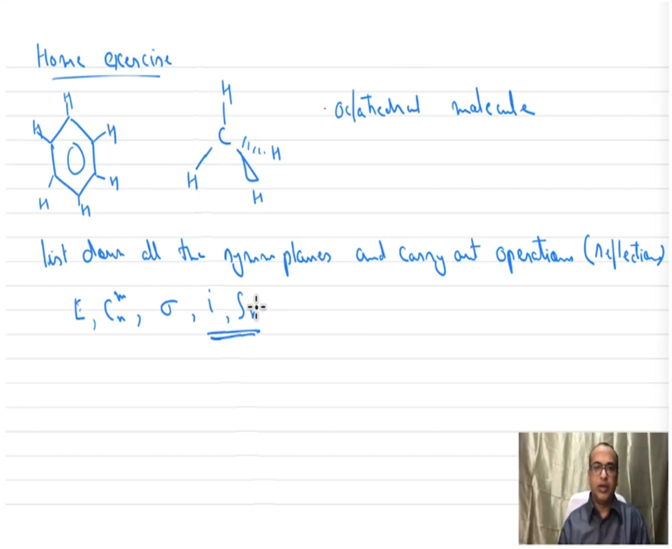

Now, let us do a little home exercise and list down the planes and do the operations corresponding operations. So, how many planes are present and then planes of symmetry are present. And then also try to do it by yourself. So, unless you actually do it by yourself by just looking at the videos or by looking at other study material, you will never be able to figure it out. While if you practice then only you will be able to figure out.

Because you actually have to sit in the molecule and see around yourself that okay what a particular symmetry element or the operation has done. So, also take any octahedral molecule. So, list down all the symmetry planes and carry out operations. Carry out corresponding reflections. So, if you can list down all the planes you will see that how easy it is, but unless you actually do it, it will be very difficult to memorize. So we are finished 3 symmetry elements E, Cn ^m and sigma. So, we are left with inversion and Sn. So these 2 will be taking up in next lecture. So that is all for today. Thank you very much.