Foundations of Computation Materials Modelling
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Symmetry Elements – 2

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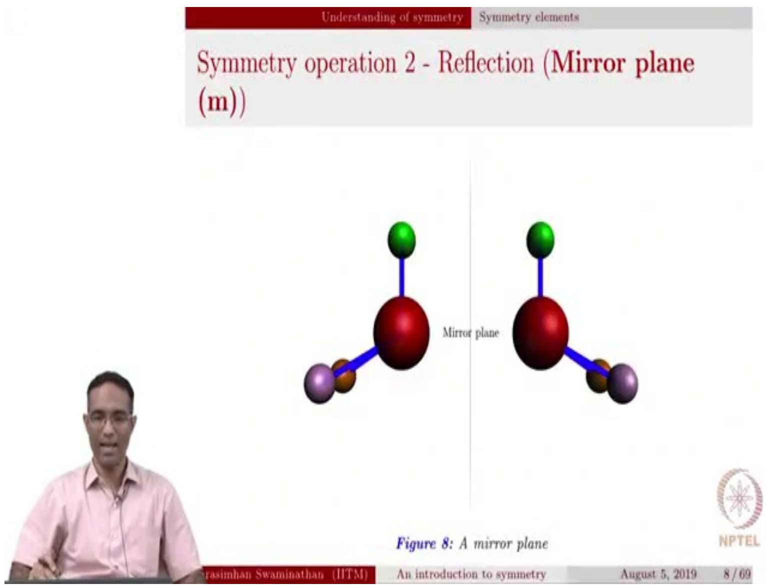

The next symmetry operator after the rotation axis which we represented by the capital X we call it capital X will be what is referred to us as the mirror plane. It is a very simple symmetry operator. So, this is a mirror plane. This molecule possesses the mirror plane. The molecule comprises of all these eight atoms one, two, three, four, five six, seven and eight. This entire molecule actually possesses the mirror symmetry.

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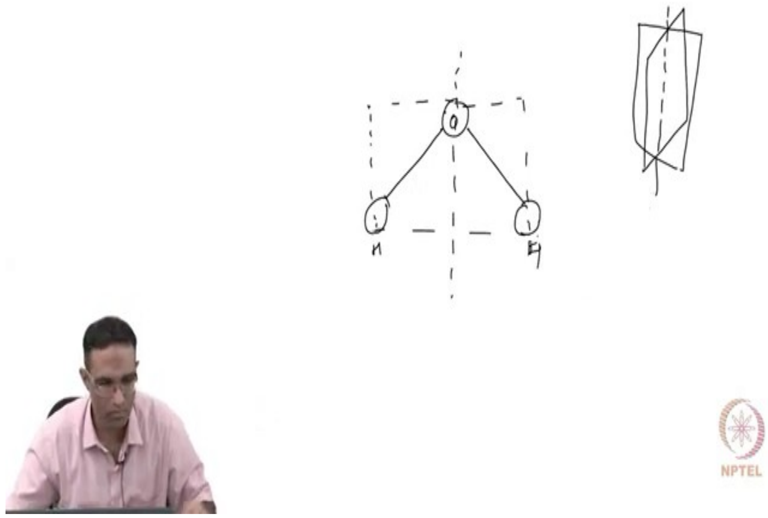

So, if you take a look at H_2O, water molecule it possesses a mirror symmetry and in addition to that it possesses something. What else does it possess? This is water molecule, this is oxygen. It has a mirror here, right? There is definitely a mirror here. There is a mirror perpendicular to the, to this tablet, like this which I represented this way and then there is also a two-fold symmetry. If I rotate it by two-fold about the same axis, this will come here and this will go there and you will not be able to distinguish.

Oxygen, Hydrogen, Hydrogen, you cannot distinguish between the two hydrogens, consequently you have a two-fold symmetry as well and you also may have another symmetry which is along the plane of this thing, so something like that a mirror which is cutting these spheres that way. There is also a symmetry element that is going to be present. Is that clear? But the presence of this mirror and the one that is perpendicular to it automatically implies that there is a two-fold symmetry.

If there are two mirrors that are perpendicular to each other, it will automatically imply that. There is a two-fold symmetry passing through the line of intersection between these two mirrors. There is a mirror like that and there is a mirror like that. There is automatically if there are two one, the presence of any two automatically implies the presence of the third one, this is something that we have to keep in mind.

So, whenever we represent these the symmetry of these elements, it may not be necessary to talk about all the symmetry elements that the particular molecule has, because you know, you will have cases where the presence of any two automatically implies the presence of the other. This is something to keep in mind.

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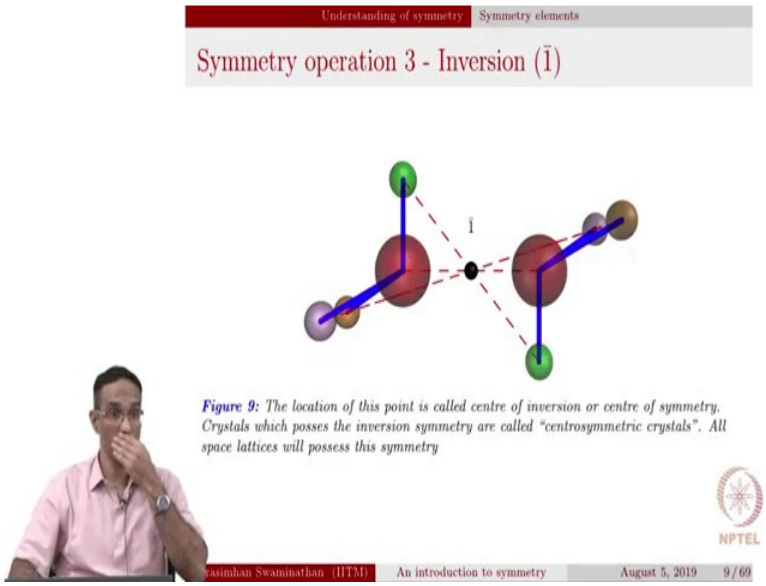

The next operation is called as the inversion. This entire molecule, the entire thing comprising of the eight atoms possesses the inversion. So, there is a point through which you can invert the coordinates of these atoms. For example, this will come to other end, this grey will go to, this one is going to this; this one is coming to this one.

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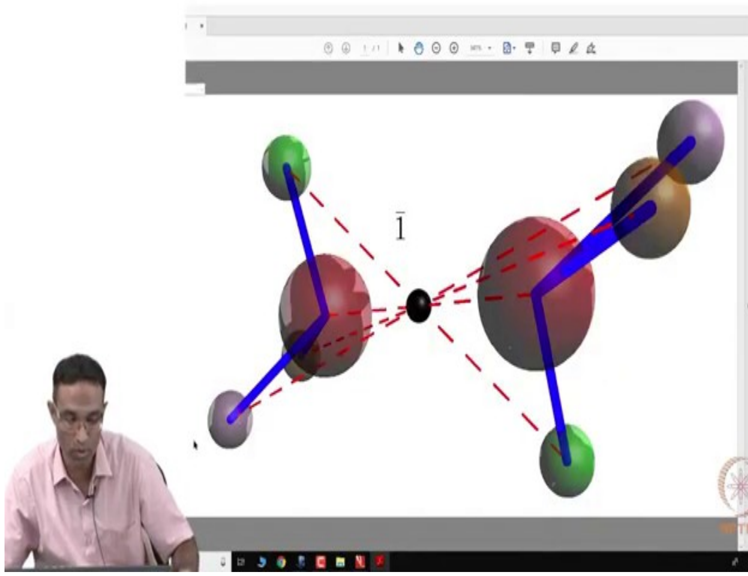

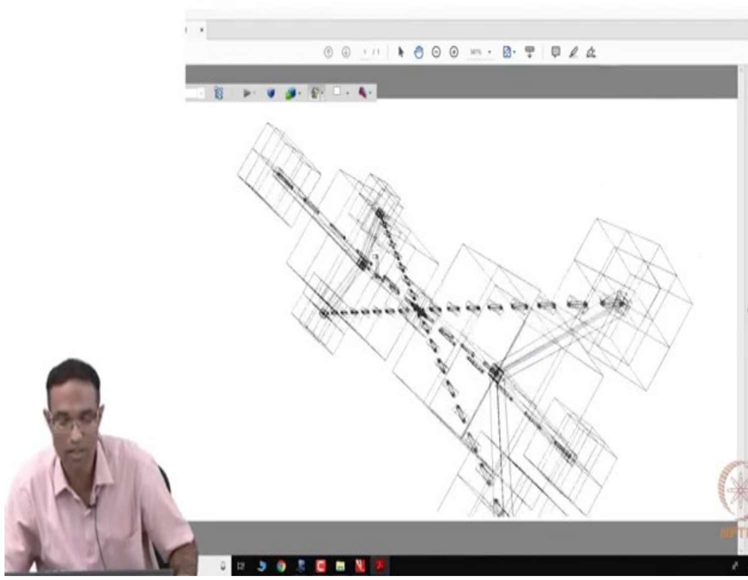

So, a three dimensional. So, you see that this grey atom is going through these black ones, this is the inversion centre, this is the centre through which I am inverting. It is going to the other end. This green one is coming here and this red one is going right there, these are called as the inversion, this is called as inversion centre.

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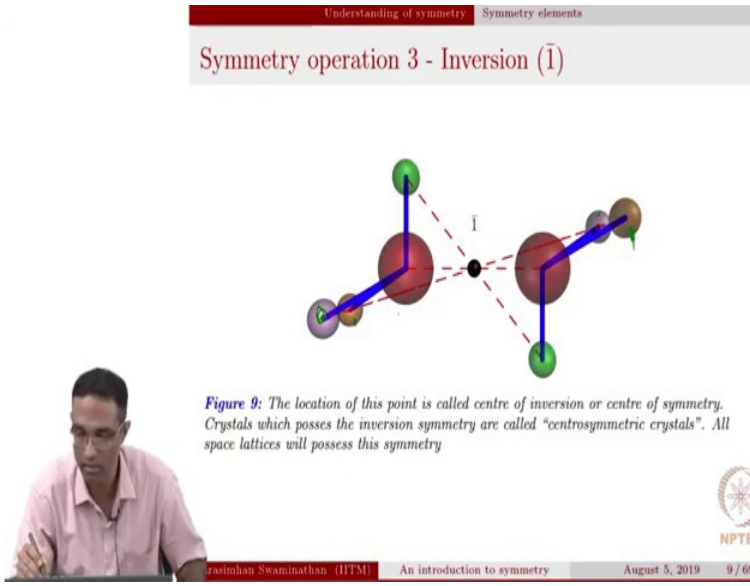

And the Symmetry element is represented by using one bar that is the symbol for the Inversion Centre. The symbol for, what is the symbol for your mirror? Just m, and what is the symbol for the axis of rotation, symmetry operator? X, the X fold or N Fold is two or three or four or six is basically the symbol. These symbols are called as, anybody knows the name of these symbols? It is not the swain flee symbol, is called as the Hermann Mauguin symbols. We will introduce those symbols in a little bit. That is very, that is a much more useful way of talking about symmetry operators.

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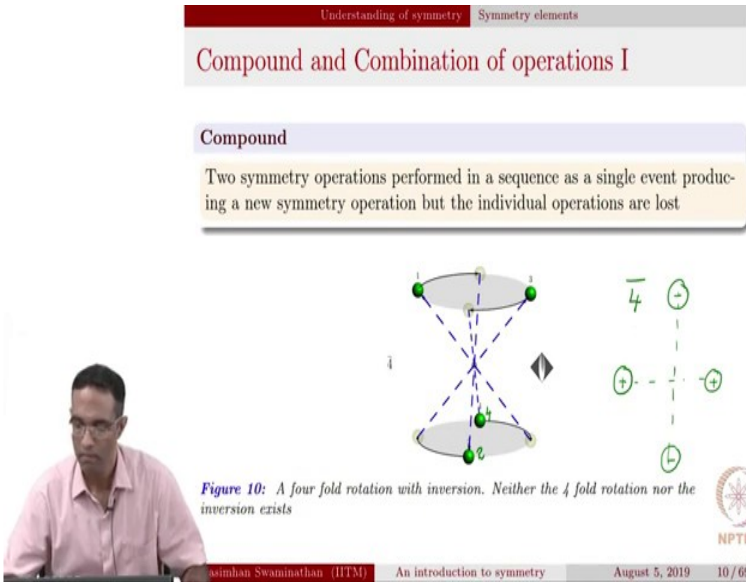

So, we talked about separate symmetry operations such as the rotation and mirror and inversion. Now, we will talk about compound symmetry operations and combination symmetry operations which involves both of them, which involves maybe two operations like rotation and inversion or rotation and mirror. So, this is an operation which is which involves a 4-fold rotation and inversion but each of the symmetry elements are completely lost. Let us take a look at this molecule.

So, one, three, four, and two are the atoms that are making up the molecule. You are able to see two right here, two? So, this is two, four, this is four, atom number four, this is atom number three and this is atom number one. Now this entire set of four atoms has the symmetry four bars. That means I perform a 4-fold rotation and an inversion, I will be able to make this entire molecule coincide with itself. Take a 4-fold rotation and invert all the atoms, you will be able to generate exactly the structure.

So how do you generate these structures? You do these operations over and over again until they start repeating. For example, 4-fold rotation, inversion I did it once. So, I started off with look at the way write it; it is the kind of going to be a little bit tricky. So, I started off with an atom which is above the plane so I put a circle and I put a plus sign. I performed 4-fold rotation but there is no atom that is going to come over there. I perform an inversion so there is going to be an atom but that is below the plane, it is below the plane, now I keep doing this again.

So, I perform 4-fold rotation on the lower plane and invert it, so I get a plus or minus?, plus very good. So, I perform a 4-fold rotation, perform an inversion, I get a minus. So, the top view of these entire thing is going to look like this, there is going to be plus plus minus minus. However, neither the 4-fold rotation nor the inversion are separately present in this molecule, what is present is the 4-fold rotation plus an inversion.

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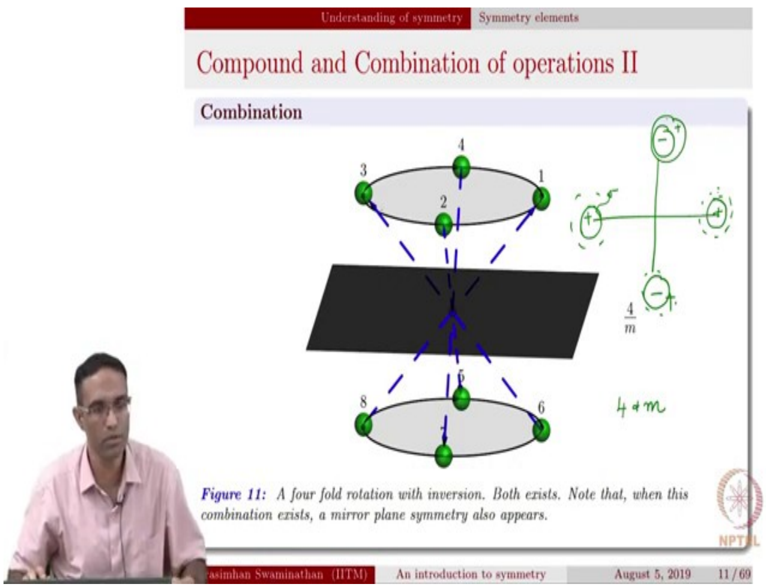

The next one is 4 over m. I am giving an example, 4-fold rotation with a mirror plane that is perpendicular to the access of the 4-fold rotation. So, it should not be too hard for you to look at this molecule. So, again how do we generate such structures for our understanding? We take one atom and keep applying the operations over and over again until we generate enough number of atoms so that they start repeating themselves.

So, let us start from one, we start from one. This is one, the top view one, perform a 4-fold rotation and mirror perpendicular to it, consequently I will generate an atom here, again a 4-fold rotation of the bottom one and then mirror plane. So, I will generate one on top, a 4-fold rotation and a mirror I will generate a minus, this is what? This plus, a 4-fold rotation and a mirror. So, right beneath this there is also going to be a atom with minus, a 4-fold rotation and a mirror plane.

So, that will be a plus; keep doing it, you will get a minus here, sorry a plus and there is also a minus and here you have a plus. So, this molecule of 4-fold rotation and a mirror perpendicular to it has both 4-fold rotation and a mirror. Both the operations are actually present when I perform this 4 over m. Are you able to see that? There is both a 4-fold rotation and a mirror. So, is there a 4-fold rotation, you are able to see? If I take the entire thing.

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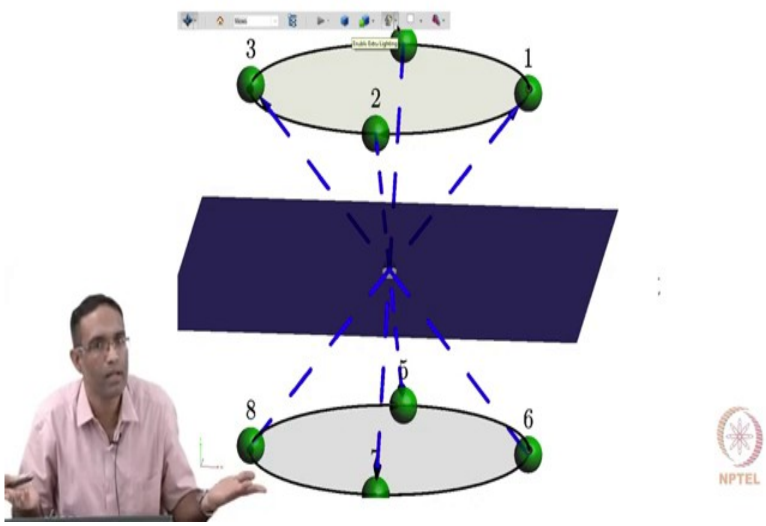

So, this is, if I take this and rotate it by 90 degrees, the entire molecule, the entire molecule involves all the eight atoms. If I rotate it by 90 degrees all the atoms are going to, one is going to coincide with four, four with three, three with two, two with one and five with eight, eight with seven, seven with six, six with five and I will not be able to tell the difference whether the operation 4-fold was performed or not. If I put a mirror perpendicular to the 4-fold rotation, three will go to eight, two will reflect with seven and whatever is here, one two three four will go to five, one will go to six.

So, 4-fold rotation and a mirror plane perpendicular to it has both four and the mirror, both of them are there, unlike the case of four bar where neither the four nor the inversion were actually present in the molecule, separately they were not present, is that ok?

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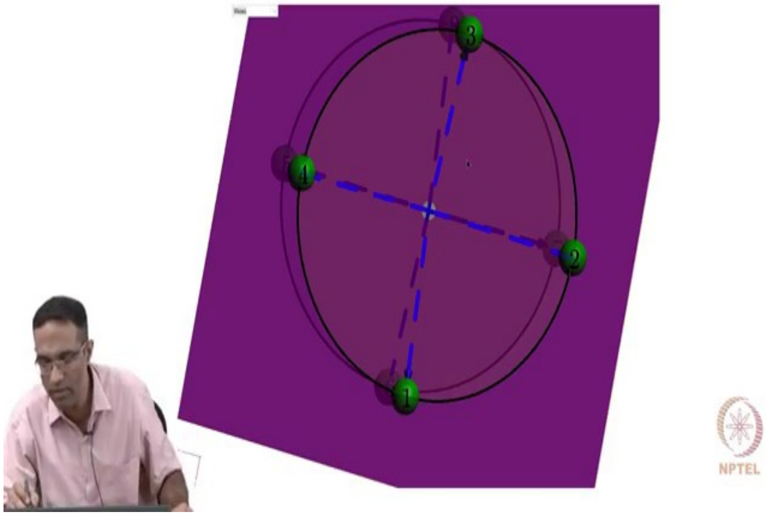

So, this is the four bore one. So, if you look at it this way both the plus and the minus atoms essentially coincide, the plane, below that you see five, below three you see eight, below seven you see two, below one you see six.

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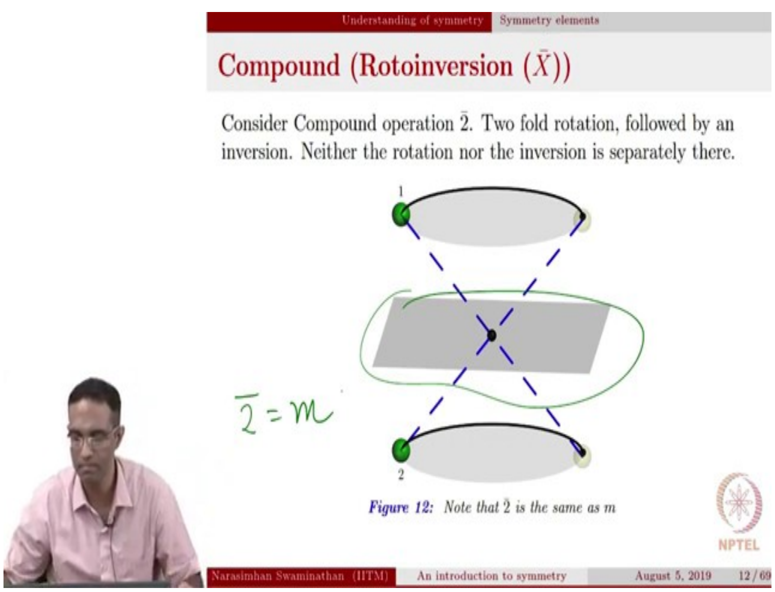

So, this is another operation called as two bar. Two bar means what? Four bar means 4-fold rotation and an inversion two bar means two-fold rotation and inversion, but you see that a two-fold rotation and inversion, neither the two-fold is present, the two-fold is not present separately for this molecule, it involves molecule, atom one and atom two, for this molecule you do not have separately the two-fold rotation. Separately you do not have the inversion also but the two-fold rotation plus an inversion is a resulting in ‘m’.

So, two-fold rotation plus an inversion is the same as a mirror plane. So, these sort of things will come a couple of times, the presence of two of these things will mean something else, consequently like I mentioned previously we do not have to specify all of them. If you knew that the presence of two means the other.