Symmetry and Group Theory

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Module No # 02
Lecture No # 07
Coordinate System and Inversion Center

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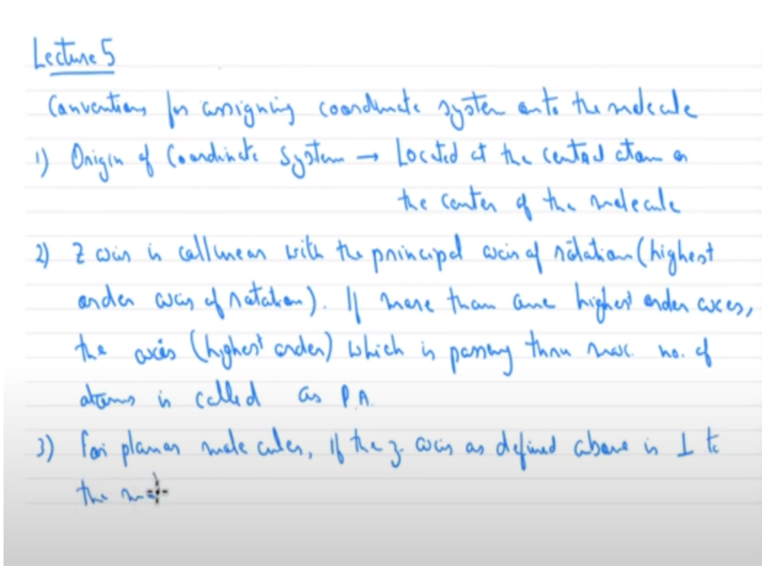

Welcome to lecture 5. So, in continuation of our discussion with coordinate system, let us so I saw that there was some confusion how to assign the coordinate system. So, let us see how to do it in an explicit manner. So, let me define the explicit rule so that there is no confusion and it is clear once for all. So, conventions for assigning coordinate system on to the molecule. So, this was initially I think covered in lecture 3 and then all the rules were not explicitly defined.

So, let see that is why I am doing it again over here. So, first of all the origin of coordinate system. So where should the origin lie? It should be located at the central atom, or the center of the molecule. Ok, so that should be easy to identify. Then second point is that z-axis is collinear with the principal axis of rotation. So, principal axis of rotation, what is the principal axis of rotation? So again, to clarify it is the highest order axis of rotation, ok.

So, for example if there is one C2 and one C4, so C4 will be the principal axis. And what is so if you have more than one highest order axes, in that case the axes of course the highest order axis, this will be i because it is singular. So highest order axis. If more than one highest axis are present, the axis which is passing through maximum number of atoms is called as principal axis ok. So now it should be very clear.

So, z-axis has to be collinear with highest order axis and if there are more than one highest order axis, the highest order axis which passes through the maximum number of atoms will be called as principal axis and z-axis will be collinear to that. Now how to define that x-axis and y-axis. So let us first define for planar molecules. For planar molecules, if the z-axis (as defined above) is perpendicular to the molecular plane.

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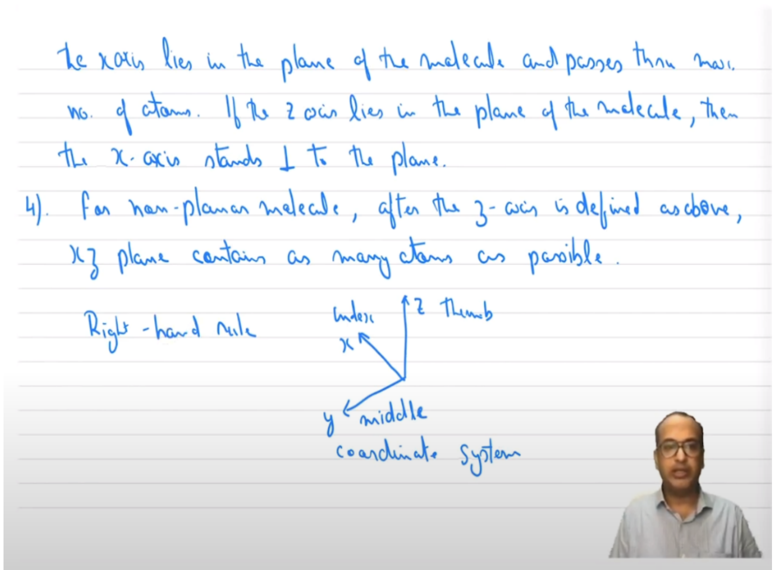

Let me go the next page. In that situation the x-axis lies in the plane of the molecule and passes through maximum number of atoms, ok. However, if this is again for the planer molecule only, so I am continuing the same point. So, if the z-axis lies in the plane of the molecule that can also happen, in the plane of the molecule, we will see an example shortly after this. Then the x-axis stands perpendicular to the plane, ok.

Now if the z-axis lies in the plane of the molecule, then the x-axis stands perpendicular to the plane. Now for non-planer molecule. So, of course, after the z-axis is defined as above, xz plane contains as many atoms as possible, ok. So, this covers all. So this should not be a problem and the convention, of course, we follow is the right hand rule. So, what is right-hand rule? So right-hand rule says that if you have this will be our z which is oriented along thumb of your right hand. And then if this is your index finger, then that goes as x, and then the middle right it is like this. So middle finger points towards y-axis. So, this is the orientation or right-hand rule which we follow for the coordinate system. So, we have to follow this one so that there is no confusion. So now let us quickly look at the example.

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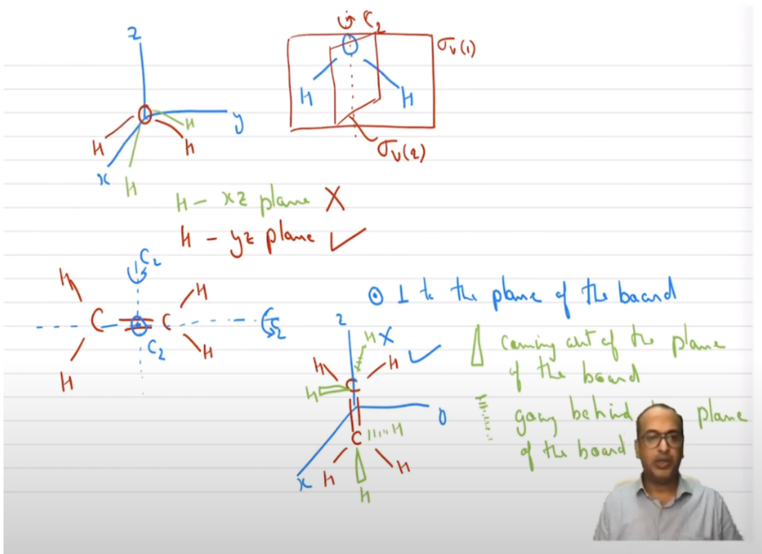

So, let us say we were discussing so right-hand rule right hand coordinate system can also be defined, can also be oriented like this. So, let us say we have water molecule, ok. So in this case where is our principal axis? Principal axis is C2 which is lying in the molecular plane right. Of course, we do not call it as sigma h in this case, this is sigma v1. Then the, another plane is the one which is bisecting the H-O-H angle and both of them are containing C2 and this one is called as sigma v2 right ok.

So, now in this case, so first of all the center of the molecule we really do not have any center of molecule. So, we will just use the center atom which is oxygen in this case as the origin, ok. And then since the C2 axis is the principal axis. So that goes along z-axis so that is how our molecules is going to be. Now whether we will define the H the 2 hydrogen’s in the yz plane like this or we define the hydrogens like this in xz plane.

So, the green hydrogens are in xz plane and the red ones are in yz plane. So, which one is the correct orientation? So now if we go back to the rules which we have stated. So, if we see this, so for planer molecules H2O is the planer molecule so we will use this condition. If the z-axis has defined above as the perpendicular to the molecular plane is it perpendicular to the molecular plane? No, it is containing the molecular plane.

So next so if the z-axis lies in the plane of the molecule, then the x-axis stands perpendicular to the plane ok. So that means the x axis should be perpendicular to the molecular plane. So that means the red orientation is the correct orientation ok. So, the red orientation is the correct one and the green one fails because of this one right over here, because of this point. Because z-axis lies in the plane of the molecule. So, x-axis stands perpendicular to the plane, ok. So, let us look at one more case. Let us see the other case which has confusion is C double bond C the ethylene molecule.

Now in this case, what is your principal axis? So, you have 3 highest order axes here. One is passing through C C double bond, which is C2. Then another is perpendicular bisecting the C C double bond, which is also C2, and the third one is perpendicular to the plane of the board and passing through this right and perpendicular to both of these C2. So, this is third C2. So, I am drawing anything to this perpendicular to the plane of the board I will draw it like this ok.

Perpendicular to the plane of the board so that it is clear. So all through I am going to use this notation for any axis which is perpendicular to the plane will be drawing like a circle and then a point ok. Now we have 3 axes which one will be principal axis. So principal axis by definition will be higher order axis passing through highest number of bonds. So that means this right here is my principal axis right.

Now principal axis has to goes along the z-axis. So, let us draw the coordinate system x-y-z. Now the center of the molecule is clearly here between the bonds. So, I am going to draw one carbon atom above origin another carbon atom below origin, and now here is my double bond right. So now where to draw the 4 hydrogens whether the hydrogens will be in yz plane like this or the hydrogens will be in let say like this H H.

So again, this notation is like if anything is any bond is drawn as a solid wedge, this is coming out of the plane of the board, and any bond which is drawn like this, is going behind the plane of the board, right ok. So now let see whether the green one is the correct one or the red one is the correct one. So green is now in the xz plane, red is in the yz plane. So, let us see the principal axis is in the molecular plane so here if z-axis lies in the plane of the molecule.

Then x-axis stands perpendicular to the plane, so in this case also our x-axis will be perpendicular to the plane that means the red orientation is the correct one ok. So that means the red one is the correct one and the green is wrong. So that is how you are going to define the coordinate system on to a given molecule. I hope this should be very clear now. I have taken 2 examples, which are particularly important in terms of they have slight confusion how to define the principal axis and so on. So that is why I have chosen these examples ok.

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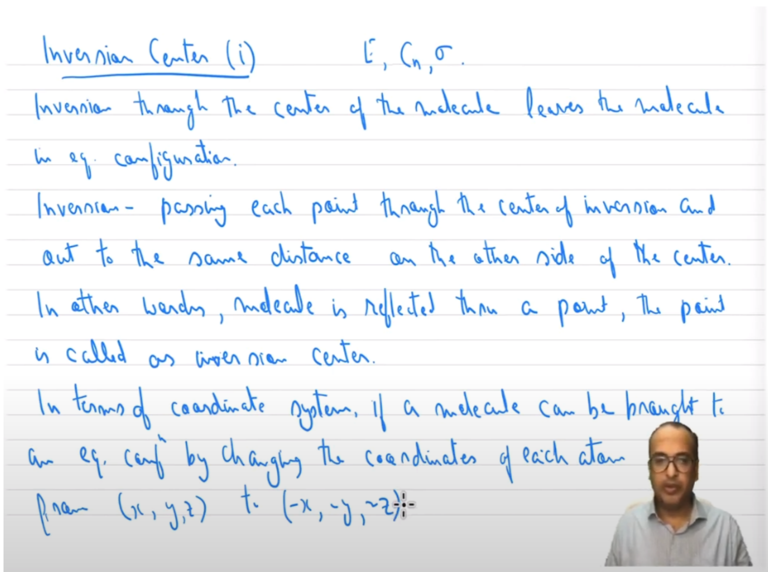

So now let us move forward with inversion center. So, this is the fourth symmetry element. So, we were discussing symmetry elements and operation right. So, this is the fourth in the series we have already covered E, Cn, sigma, and now we are covering i, inversion center symbol is i. So, what is this symmetry element? The symmetry element is defined as inversion or symmetry operation is defined as - inversion through the center of the molecule leaves the molecule in equivalent configuration, ok.

So that should not be a problem to understand. So how do we do that? So, let us say, inversion - passing each point through the center of inversion and out to the same distance on the other side of the center that is the operation. And if you get an equivalent configuration you say that the molecule has inversion center otherwise it does not, ok. So, we can also say, in other words, molecule (technically it is not a reflection but you can say that) molecule is reflected through a point. I mean you need a surface to reflect but this is colloquial definition.

So, in other words you say the molecule is reflected to a point. The point is called as inversion center. So, in terms of coordinate systems, coordination system in terms of coordinate system, so if a molecule can be brought to an equivalent configuration by changing the coordinates of each atom from let say general coordinates are (x, y, z) to (-x, -y, (basically changing the sign) -z).

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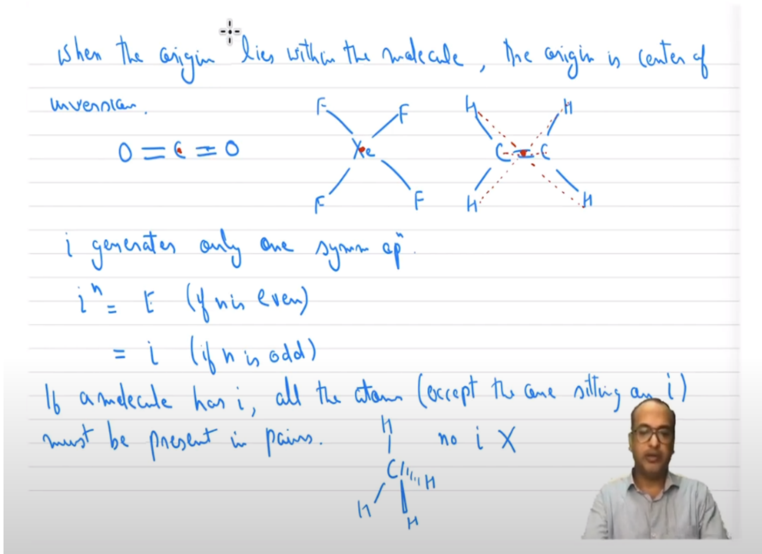

When the origin lies within the molecule, the origin is center of inversion or inversion center, either way is fine, alright. So, let us look at an example, for example if you have CO2. This will be your, Carbon will be your inversion center right. So, because if you, see oxygen 1 will be replaced with oxygen 2 if you reflect everything from this point. Similarly let us say if you have XeF4, again the center of this molecule will be the center of inversion right.

Similarly, let us say we have just discussed ethylene. In this case, the center of this bond will be the inversion center. So, for example if I am going to draw a line through this and extend it further, it will meet the same atom. Similarly, from here if I do this, it will meet the same atom at the end. Similarly, for carbon it will do this, right ok. So now how many operations it generates, because number of operations are also important.

So i generates, yes you guessed it right, only one (just like sigma) symmetry operation. So that would mean i to power of n will give rise to E if n is even. And i to the power n will give rise to i if n is odd ok. So, one important conclusion from here, if a molecule has i all the atoms, except the one sitting on i, must be present in pairs right otherwise you will not able to reflect one atom with other atom of same species. So, that means we do not need to look for an i inversion center which has odd number of atoms of more than one species.

So, if there are 2 different species which are present in odd numbers that means the molecules cannot have i, right. But vice versa is not true. So, for example tetrahedral molecules so if you have CH see you have hydrogen in two pairs carbon is in single number. But still, this does not have i, so no i here right. So vice versa is not true but the other way round it is true. So, if your molecule has i all atoms must be present in pairs except the one sitting on i.

So, you can see here for example the fluorines are present in pairs. Whereas the one which is sitting on to the i is not present in pair. Similarly, here because there is no atom is lying on the i so everything is present in pairs. Here also it is the same case the oxygen is present in pairs while carbon is sitting on to the i is present as the isolated atom. So, this discussion should be very clear ok. So that finishes the fourth symmetry element inversion center and in next class we will see improper axis and improper rotation, ok. So that is all for today.