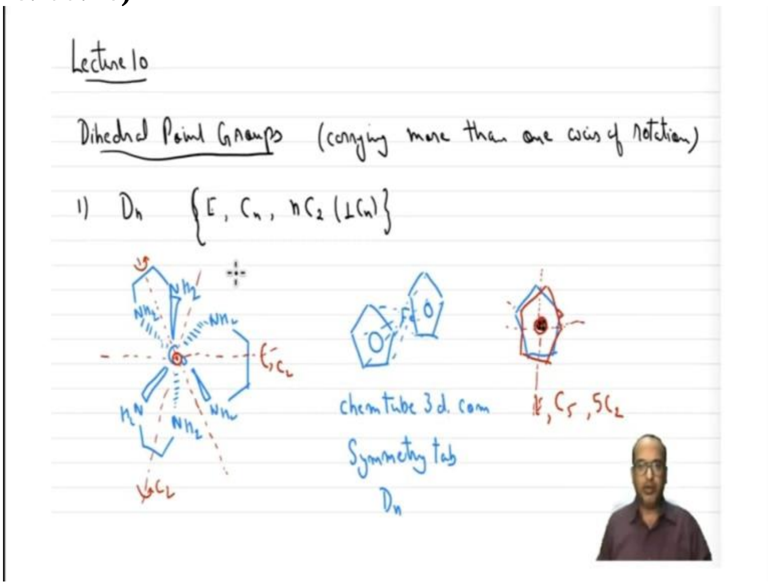
Symmetry and Group theory

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

Lecture - 14
Symmetry Point Groups

(Refer Slide Time: 00:16)



Welcome back. Let us start lecture 10. So, we were discussing symmetry point groups and, in that discussion, we have already covered single-axis rotation point groups and no-rotation point groups, right. So, now let us look at next in the category is dihedral point groups. So, what are dihedral point groups? So, basically dihedral point groups are carrying more than one axis of rotations. So, carrying more than one axis of rotation, so you can immediately think of many examples that we have already discussed.

So, let us look at it one by one. So, the first category is within dihedral point groups, the first category is Dn, so typical elements will be E, Cn, nC2 which are perpendicular to Cn. So, let me use the other bracket. So E, Cn where Cn is a principal axis, and nC2s which are perpendicular to the principal axis. So, the example is, let me show you. So, this is cobalt atom, which is the central atom here and then we have tri-ethylene diamine, which are arranged something like this.

So, let me see an NH2, NH2, so it is clear that 3 NH2s are coming out of the plane of the board and 3 of them are going back to the plane. Where cobalt is sitting in the plane of the board and then these are connected with diethylene group. So, you have this and you have this. So, you can easily see that that central cobalt atom actually has the octahedral geometry, but because of this diethylene group this actually is, does not belong to octahedral point group, but Dn point group.

So, you can see that, where is your C3 axis, there is a C3 axis which is going like this. So, which is going through the plane of the board, perpendicular to the plane of the board and which will be rotating these NH2 groups 1, 2, 3 and then 4, 5, 6 and then there will be 3 C2s which are perpendicular to this C3. So that means there will be a so can anyone tell. So, you can think of maybe, so you will have 1 C2, which will be, so, this is now in the plane of the board. So, if I do this rotation. This NH2 will come to this place and this NH2 will go to this place.

So similarly, you have another C2 like this, and third C2 will be like this. So, that is one example. Then we have another example, which is called as ferrocene. So, ferrocene is molecule with 2 5-membered rings with an aromatic character and then a central metal, which is Iron and now the second ring is not exactly eclipsed, or staggered with this one but there is a slight angle to it.

I will just draw it like this and then there is coordinate bonds. So, I understand that it is not clear so because it is a 2D plane. I request you to go to chemtube3d dot com and under symmetry tab, find this molecule under Dn point group, or D5 point group. So, maybe other way of drawing this molecule will be, let me show you so is something like this and then let me draw the other ring as in colour red. There is a slight angle to it. I hope we can all see right now.

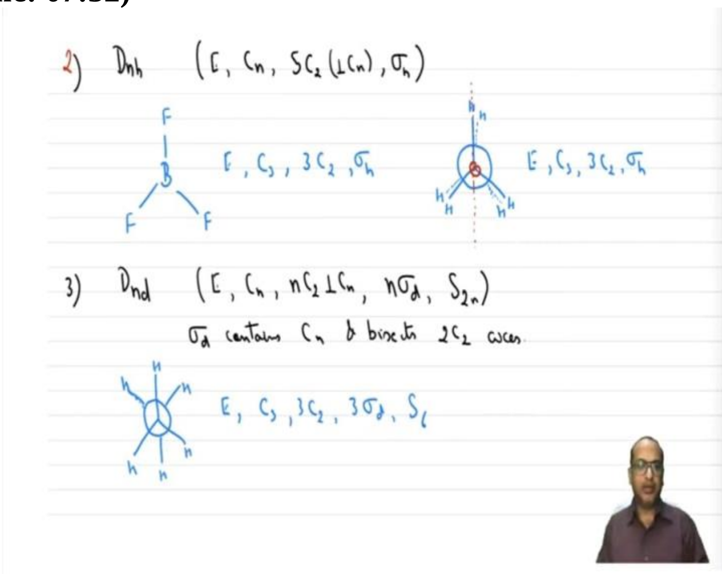
And then, so red is behind the plane of the board and blue is in front of the plane of the board and in the centre, Iron is sitting, which is in the plane of the board. So, this is here Iron. So now if you see that there is where is your axis, C5 axis is passing right through perpendicular to the plane of the board. So, you can draw it like this and then you have 5 C2s which are perpendicular to this. So 5 C2s will be bisecting through this. One similarly, we will have another C2 bisecting through this.

You can see that the 1 carbon atom is slightly to the right. The one which is behind and the one which is in front, slightly to the left. Similarly, here so you have one carbon atom slightly to the left and another to the right and C2 is passing right through between and similarly here.

So, you have 5 vertices, so 5 such C2s. So, it basically it has C5, 5 C2s which are perpendicular and E.

So, this example can be very well understood now. And if you cannot visualize it in 3D here, I request you to go to chemtube3d dot com and try to visualize the molecule there they. Both the molecules are listed in that website and it will be easier for you to understand. So, this is one of the dihedral point group.

(Refer Slide Time: 07:32)



Now, let us look at the second dihedral point group, which is Dnh. So, as the name suggests, so it will have E, Cn, again 5 C2 which are perpendicular to Cn, and in addition to that there will be a sigma-h. So, in the previous case there was no h, so h is denoted as Dnh here. Now we have already seen this example. One of the examples is BF3. So, we know that there is a E. We should be able to locate C3. So, I will not spend time on that and then we have 3 C2s and we have sigma-h. So that is very very clear.

Sigma h is the molecular plane in the plane of the board, C3 is the perpendicular to the plane of the board and then C2s will be passing through 3 B-F points. So that should be very very easy. Then we also have seen, or we have not seen, but let us see eclipsed ethane. We have seen the case of staggered ethane. When we were discussing S6 axis. So, in this case, let me draw the one with a slight angle but there is actually no angle to it. It is right behind. It is unlike twisted ferrocene and twisted ferrocene had a small angle.

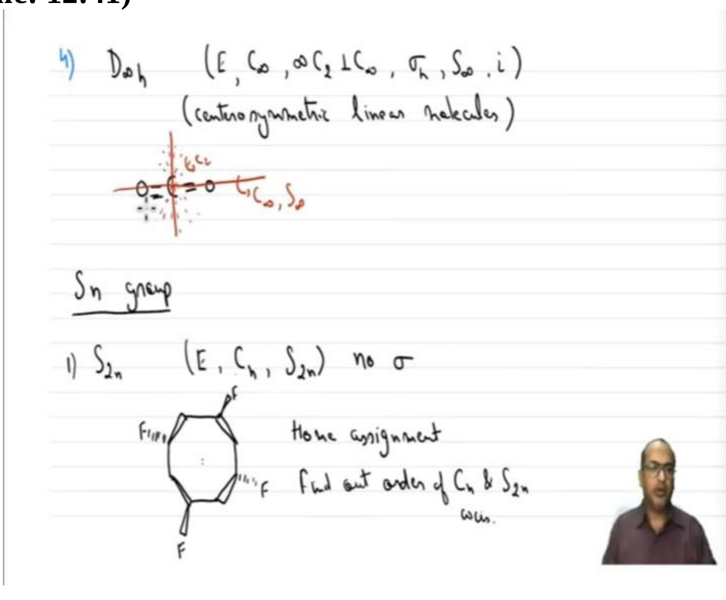
But this one is the dotted line is right behind the solid line, you have a H, H. You know how eclipsed ethane would look like. so now here, this thing would also have E, C3, 3 C2s and sigma-h. Now here the C3 would be passing through C-C bond. This one will be a C3. Then 3 C2s, will be bisecting the C-C bond and will lines somewhere in between the 2 hydrogens. So, like, it is not passing through C-H bond. It is actually bisecting the C-C bond.

It is in the plane of the board while 3 hydrogens and this carbon is actually in front of the plane of the board and the other methyl group is in the back of the plane of the board. While the 3 C2s will be in the plane of the board and sigma-h, also in the plane of the board which is bisecting the C-C bond. And then, in addition, it will have some other planes, so but these are the minimum criteria for having Dnh.

For example, this one also has sigma-Vs or sigma-Ds. This one will also have sigma-V or sigma-D. But let us not worry about this. This is the necessary and sufficient condition for it to fall into Dnh category. Now let us see the next category in dihedral planes, which is Dnd. So, Dnd has E, Cn, n C2s perpendicular to Cn, and n sigma-D and in addition, it also has a S2n. So, sigma-D contains Cn and bisects 2 C2 axis, that is as per the definition of sigma-D.

Now an example, we have already seen this example, we know staggered ethane, so I will just quickly draw it. So, we have already discussed this example so we will not cover this in detail. So, it has E, C3 we know it has C3. It has 3 C2, has 3 sigma-D and S6. We have seen how there is a S6 in this one, that we have already seen.

(Refer Slide Time: 12:41)



So, let us move ahead. And the next in the category is, D-infinity-h. So, the elements and the corresponding operations will be C-infinity. This is actually very easy to identify. Infinity C2s which are perpendicular to C-infinity, and then we have sigma-h, there is S-infinity and there is i and the typical characteristic of this molecule is that they are centero-symmetric linear molecules.

So, linear molecules can either be non-centerosymmetric or centero-symmetric. There are only 2 options we have already seen, C-infinity-v, which is non-centerosymmetric linear molecule so this one is centrosymmetric linear molecule and typical example is C double bond O, C O 2. So, the centre of symmetry lies at the carbon and then you have 2 oxygens at the end, so you can easily see where is your C-infinity axis C-infinity axis passing right through the O-C-O bond.

Then you have infinity C2s perpendicular to this. So, axis perpendicular to this so you will have one axis, another axis, another axis, there will be infinity such axes, passing through perpendicular to O-C-O bond and so on. Each of this will be a C2 axis and sigma-h. There is one sigma-h, which is perpendicular to the plane of the board and cutting, right like this. Then you have S-infinity and i, which is also very easy to see.

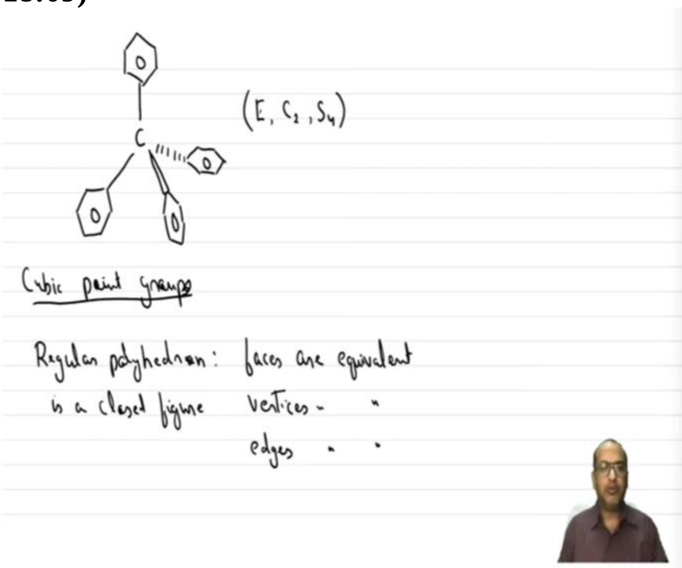
S-infinity will be the axis co-linear with C-infinity, S-infinity, i will be at the centre. So, the molecule is very easy. Centero-symmetric linear molecules will always be of D-infinity-h point below. That finishes dihedral point group. Let us now look at next category next category is very simple, but the examples are difficult to find in this group, S2n group. So, within S2n, it is actually called as not S2n, it is called Sn point group.

So, within Sn, let us see an example of S2n, there is only one category, S2n for even n basically. This will have E, Cn, and S2n symmetry elements. There are no other symmetry elements present, no sigmas. So typical example, that is actually the tedious to draw, let me see if I can draw it correctly. This particular bond is coming out of the plane of the board. And so is this one, every alternate bond is, so it is something like chaired form of cyclohexane. But this is cyclooctane.

And then you have 4 fluorine atoms attached to it, which gives it asymmetry. We can have any atoms basically here. So, you can see now, there is no sigma present to this. Because if you even, if you try to draw sigma cutting, let us say this one, will not be able to reflect the opposite atoms here. So, there is no sigma, very clear. There is E and there is Cn. So, in this case what will be your Cn.

Try to find out and then you will have a S2n. So, try to locate Cn, try to find out the order of Cn and S2n, in this case, let us take it as home assignment and if you have any difficulty, come back to me. So, find out order of Cn and S2n axis in this molecule.

(Refer Slide Time: 18:09)



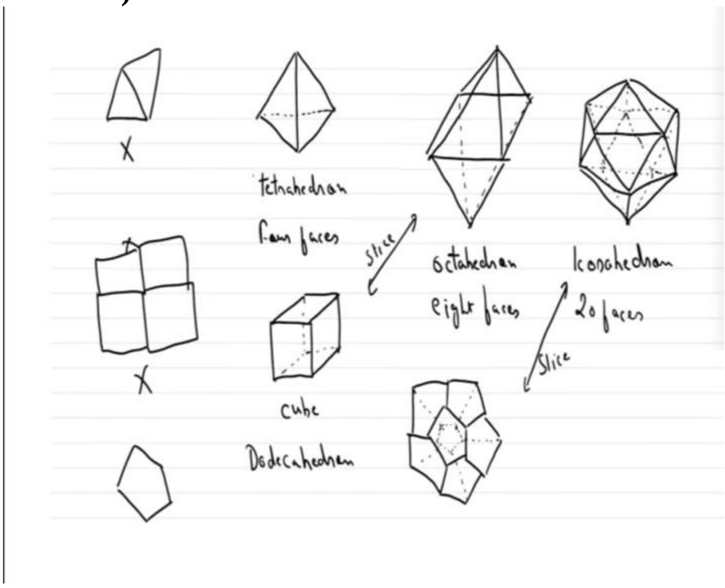
I have one more example for Sn point group, which is also a little difficult to draw. Let me see if I can draw it correctly. So now the phenyl ring, there are 4 phenyl rings connected to it. But these are not in plane exactly. This one is something like, half of the ring is coming out of the plane of the board and half of ring is going back to something like a propeller, similarly this one also.

So, here in this case I will tell you what order is E, C2, S4 it is easy to identify. So, this one is also S2n point group or S4 point group basically. So, this should be very very clear, so we have covered single-axis, non-rotational, dihedral, S2n. And last, in the category of point groups, is called as cubic point groups. So, these points groups, these are little special, special in the sense that they are formed by something called as regular polyhedra. The shape of these molecules is can be represented by a regular polyhedra.

So, let us first try to understand what is the regular polyhedra or polyhedron. So, what is the regular polyhedron? Regular polyhedron has, let me, one of my figures. Yes. So, the faces are, regular polyhedron is a closed figure, the face of each polyhedron, are all the faces are equivalent, vertices are equivalent. When I say equivalent, I mean that they are equivalent when you operate them by symmetry operations.

So, all the faces are equivalent all the vertices are equivalent and all the edges are equivalent. That means you can replace any edge by another edge by doing any kind of symmetry operation and there should be equivalent. How do you form the regular polyhedron? Let us see that. So, what it takes to form regular polyhedron.

(Refer Slide Time: 21:11)



So, for a polyhedron to form, you need to start with a equilateral triangle. Let us say if we start with the equilateral triangle, how many equilateral triangles do we join together at a given vertex, so that it can form a non-planar geometry. Let us say if we have, if we join 2 of them, then it will form only a planar geometry. So, it has to be more than 2. More than 2 meaning, this will not form a regular polyhedron.

However, if we have 3 equilateral triangles, connected. So, 2 are depicted on, 1 on this side and other on this and let me draw a little bigger, so that you can visualize it clearly. So, this is 1, This is second and the third one is at the back. This is your, this is my 1 triangle, 1 equilateral triangle. Then I have second equilateral triangle, and third one is at the back. These are the 3 which are meeting at this particular vertex and then the fourth one is automatically goes at the bottom of this, which will seal it and make it as a closed figure.

So, what is the geometry of this, this is basically a tetrahedron geometry or you can call it as tetrahedron. Now, so we combined 2 equilateral triangles along the edge, you cannot do it or at the vertex, so you cannot make a closed figure. If you combine 3, you can make a closed figure and this is a regular polyhedron. If you see, all 4 faces, it has 4 faces, which are all equal. How many edges are there? 1, 2, 3, 4, 5, 6 edges. All 6 edges are equal. All 4 vertices are equivalent. That forms a regular polyhedron.

Now let us say, if we combine these equilateral triangles, if we combine 4 equilateral triangles, at a vertex. So that will give raise to How do I draw it? Let us see, it will be easier to draw. You can see that now there are 4 faces on the top, 4 equilateral triangles on the top and 4 equilateral triangles at the bottom. So, this forms the octahedron. This also is a closed figure. It has 8 faces.

Now similarly if you draw 5, here at a given vertex 4 equilateral triangles are meeting, one is at the back, one is at the front. You have one at this side and one at this side. You have 4 and similarly 4 at the bottom. So, at a given vertex, any given vertex there are 4 equilateral triangles which are meeting. So now let us see if we can go to 5 equilateral triangles and we can make a closed figure.

So, let us try to draw it. So, so far we are playing only with triangle. Then we will have to go to the higher polyhedral. See, if we are drawing it correctly, anything which at the back, I draw it in the dotted line, so that it is not confusing. If you notice at any given vertex, there are 5 faces which are meeting. 1, 2, 3 and then you have 4 more. This one will be meeting; Let us draw this little bigger. Imagination is the key here.

Now if you see at each of this vertex, there are 5 equilateral triangles, which are meeting. Let us try to count. Let us say, if we are looking at this vertex so you have 1, 2, and 3 sides and then 4, and 5. So, pick up any vertex, here also it is easy to see at this one. We have 1, 2, 3, 4 5, Similarly, here we have 1, 2, 3, 4, 5 and here 1, 2, 3, 4, 5. So, this particular figure is called as icosahedron and here you have 20 equilateral triangles or 20 faces are forming. And this one is also a regular polyhedral, it falls into the definition of regular polyhedron.

Let us also see, if we try to combine more than 5 equilateral triangles at a given vertex, you cannot form, you can try, you cannot form a regular polyhedral. It will not fit into a regular geometry. These are the only possibilities which can be formed by a triangle or equilateral triangle. Let us also look at what can we do with a square.

If we have a square, if we combine 2 squares, you cannot do it. If you combine 3 squares, you still cannot do it. So, you have to, no, you can do it actually with 3 squares. You can do it. But how do you do it? How do you do the 3 squares, will actually form a cube. Here if you see at each vertex, there are 3 faces, which are connected. At each given vertex, there are 3 faces which are connected, so this also forms a regular polyhedral.

And this one is easy. This one you know that is a cube and if you try to combine 4, these things at a vertex, then it will form a planar structure again. It will no longer form. This is also not a possibility. With square, the only possibility is the cube with a triangle, there are 3 possibilities. Now let us go to a higher polyhedral even higher polyhedral so let us go to 5 sides, a regular pentagon.

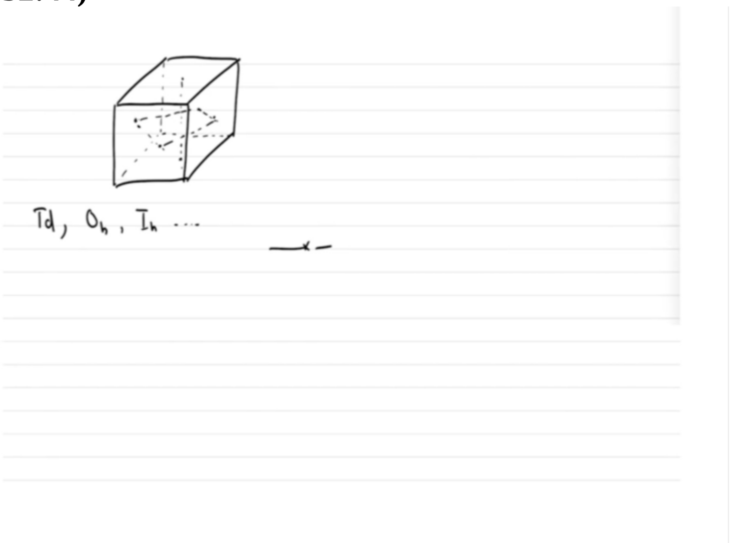
If we try to do it with a regular pentagon, you end up forming the, something called as dodecahedron. How do you draw it? It is actually easy if you see that if you slice the vertices here, I just try to do it for you. If you slice the vertices here, you will end up in a pentagon. So, all these vertices if you slice at equal lengths, you will end up pentagons joining each other. Let us try to draw it, so that it is clear.

Now, try to draw 5, all of them connected with each other, we have 1, 2, 3, 4 and this one is fifth. Drawing the 3D figure on 2D is sometimes a problem. Let us see and then you have at the back, each of this is connected. Now you see that at each vertex, at a given vertex, there are 3 phases. 1 phase, 2 phase and third phase. At each given vertex that there are 3 faces. Similarly, here, we see that 1, 2, 3. If you see it here 1, 2 3. So, there is an interesting relation actually, if you slice this one, at along the vertex, you will end up in icosahedron.

This thing is related to this thing with slice operation. It is not a symmetry operation. This is just for understanding. This is related with a slice operation. Similarly, if you cut a cube, along the vertices, you will end up in octahedron. This one is also connected with a slice operation, so that means these 2 will have same point, because you can fit octahedron inside a cube or you can fit cube inside octahedron, without actually worrying about the symmetry.

Similarly, icosahedron can be fit into dodecahedron and dodecahedron can be fit into icosahedron. So, I will try to draw it a little quickly and then we can stop for today.

(Refer Slide Time: 32:44)



Let us see, if you have a cube, you can see that how the 6 points at centre of 6 faces (incorrectly spoken as edges) will actually form octahedron geometry. It is very easy to see. Similarly, within octahedron, you can fit a cube. So, this leads to a set of point groups called as cubic point group. The name is cubic but it has non cubic entities also. So, the point groups are, we will see in more details later on in next class, but I will just list down.

Tetrahedral, octahedral, icosahedron and so on. We will see a little more detail of it, but I hope it is clear that how these regular polyhedrons are formed, so any molecular shape, which is related to these shapes can be categorized into these point groups. why understanding these shapes are important because these are very highly symmetric point groups and the number of operations are huge and it is difficult to list down all the operations at times

But if you know that the molecular shape is closer to any of these shapes, you can immediately identify and then you can try to locate all the point groups. So, that is all for today. Let us continue in the next class with more details of what are the symmetry elements and operations for these point groups and what are the other categories within cubic point groups. Thank you very much.