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

Lecture - 15
Tutorial 3

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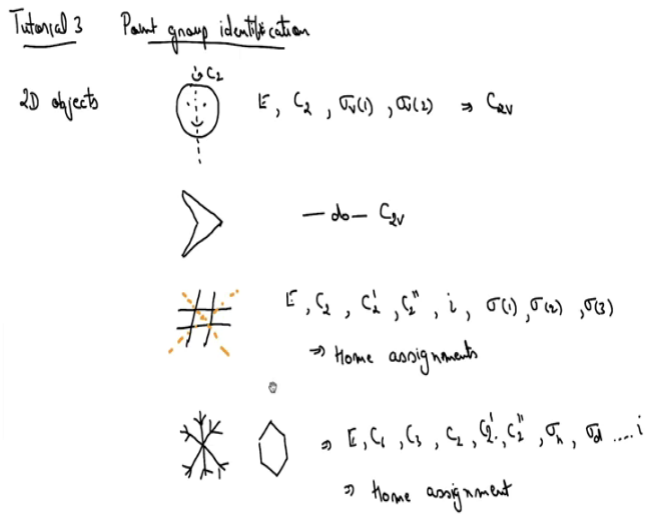

So welcome to the third tutorial of this course. So, in this tutorial, we will be learning how to identify point groups. And we will take different solved examples, we will take 2D objects, we will take 3D objects and also take different molecules. So, let us start this tutorial. So, identifying point group is very, very important for this course. So, you must need to learn very, very carefully that how to identify point group of a molecule because rest of the course totally depends on this particular step.

So, let us get this going. Tutorial 3. And today we will be discussing point group identification. So basically, what we need to do is we need to identify what are the symmetry elements present? And what are the corresponding operations, right? Given a range of different things and what happens if we distort a molecule? How does the point group change and so on, so forth? So, let us say if you have, so let us we will start with 2D objects, random objects we will choose?

So, let us say if you have a smiley face, it is a circle with 2 eyes and a smiley. So, what do you think the point group of this will be? So, if we try to list on the elements, we have E, and we have a C2 which is passing through the center, like this. So, you have I am not going to draw for all the molecules, I am just mentioning it for the sake of this first molecule. Now, it is a sigma-V1, and we will have sigma-V2.

So, sigma-V1 will be the plane which is perpendicular to the plane of the board and carrying C2 and sigma-V2 will be the plane which is in the plane of the board and also carrying C2. So, this is the case like water molecules. So, you have C2v point group? So, that was easy. So now let us look at another drawing like this. So, what we have today is arrowhead something like this, not the complete arrow just the arrowhead.

So, here we had smiley, now we have arrowhead. So, arrowhead also has the same set of symmetry elements if you notice, so, you have a C2 running through like this and then you have sigma which is in the plane of the board, sigma which is perpendicular to the plane of the board both carrying C2. So, again the point group will be C2v. So, that is easy again. Now, let us look at hash sign. So that can get little tricky. What is the point group here?

So, hash sign, consider that these lines are parallel and slightly angled to this one. So, the vertical lines are not completely vertical at a certain angle, let us say the angle between this is 80 degree or something. So, now what will be the point group. So, if you notice that you have a C2 which is perpendicular to the plane of the board passing through the center, then you have another C2, which is bisecting these 2 are like this, let me just draw it.

So, you have one C2 like this, another C2 like this, another C2 like this. So, you have 3 C2s and all 3 of them are perpendicular to each other. So, you have E, C2, C2 prime, C2 double prime or you can also say 2 C2s, which are perpendicular to one of the C2. So, you have C2 prime, C2 double prime, what else do you have? Do you have i here? Yes, we have i. What else do you have?

You have 3 sigmas, each of the C2 will be containing 1 sigma. So, you have sigma 1, sigma 2, now, this will be sigma-h so, I am just writing sigma you can say sigma-V1, V2, V3 and so on or D1, D2, D3. So, now this goes into what kind of point group or any ideas so, let us leave this to you as a home assignment. Now, we have listed this elements your job is to find what will be the point group.

Now, let us take another example. So, what we have is a snowflake. So, snowflake is, it looks something like this. Now, if you carefully see that it will have a C6 axis, it is almost like a benzene case. So, it has an order 6 symmetry. So, it will have C6 axis which is perpendicular to this, i, sigma h, and so on so forth. So, what will be the point group so, you have E, C6, C3, C2, then there will be C2s which are running in the plane of the boards, and you have sigma-h, and you will also have sigma-Ds and so on so forth you will also have i.

So, again what will be the point group here? So, I will ask you to do that, so, try to work it out. So, similar to this the way I have picked up a few shapes, try to look around where you are living or where you are studying, pick different objects and try to find out what point group does it belong to. So, that that will give you some practice of how to identify a point group of objects or a molecule.

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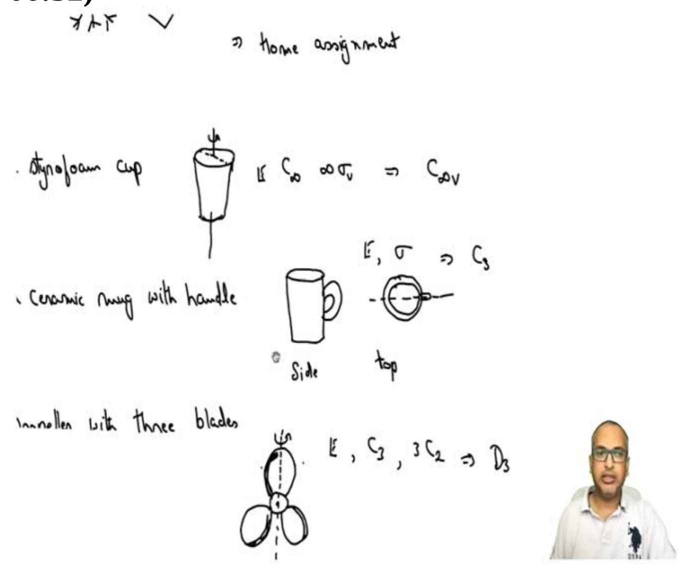

Once you know how to find out point group of an object, the molecule will also be an easy case. So, these were 2D objects. So, let us look at some 3D objects. So, the first example I have here is Styrofoam cup. I typically if it is an offline class, I typically carry these items so that it is visible to all of you, but in an online class I can only draw but you should be able to imagine how a styrofoam cup looks like.

So basically, you have a, it is not a right circular cylinder it is something like this. So, you have a styrofoam cup, which is used to drink tea, a portable cup. Now, what will be the point of this. So, if you think that if you bisect or if axis, which is going to the center of this will be what kind of axis this will be this will be C-infinity-axis. And if you now take the planes, which are bisecting in the middle and containing this axis.

So, these there will be infinity such planes, which will be all of them will be sigma-Vs and of course, you have E. So, this basically is like an HCl molecule. So, you have a C-infinity-v point group. So, that is easy. Now, let us say if we had handle to this, so, now a ceramic mug, which you used to drink coffee, let us say mug with handle. So, how does it look to you have now this is like a let us say you have a right circular cylinder kind of thing and you have a handle.

So, and from the top if you look it looks something like this. So, this is a view from the top this is from the side. So, now what will be the point group here? So, let us list down the elements. So, you have E what else do you have? Do you have any C2 here? any rotational axis? you do not have any rotational axis because of this handle destroying the symmetry? So, all you have is 1 plane which is passing through this.

So vertical plane which is passing through this so you have sigma, so the point group will be Cs. There is no other symmetry element or operation. So that is easy. Likewise, you can pick up any object around you and try to work out different things. Now let us say if you have a propeller, you must have seen a propeller like for example exhaust fan in your home. So, propeller with 3 blades.

How does it look? So, you have a circle which is the center of the motor and then you have a blade kind of thing, where some part of the blade is coming out of the plane. So, let us draw that thick and this part, let us say is going behind the plane of the board. Likewise, that is how it will propel all the blades will not be in the plane of the board? So, they will be like there will be a little twist to the blades, that is how it will propel.

So, now what will be the point group? What all symmetry elements it will present it will contain. So, you have E, then you will have C3 passing through the center and perpendicular to the plane of the board and you will also have 3 C2s. Now, the C 2s will be bisecting each blade like this in the plane of the board. So, half of the blade is coming out of the plane of the board half of the plane is going below the plane of the board.

And when you do this rotation this half goes there and this half comes here and similarly, this thing also is reflected. So, this is how it will have 3 C2s. So, that means, there is no other plane or anything any other symmetry element. So, this will be a D3 point group similarly, you can have propeller with 4 blades, so, then it will be D4 point group, and so on and so forth. So, propeller with 3 blades. So, now, this is for 2D and 3D objects.

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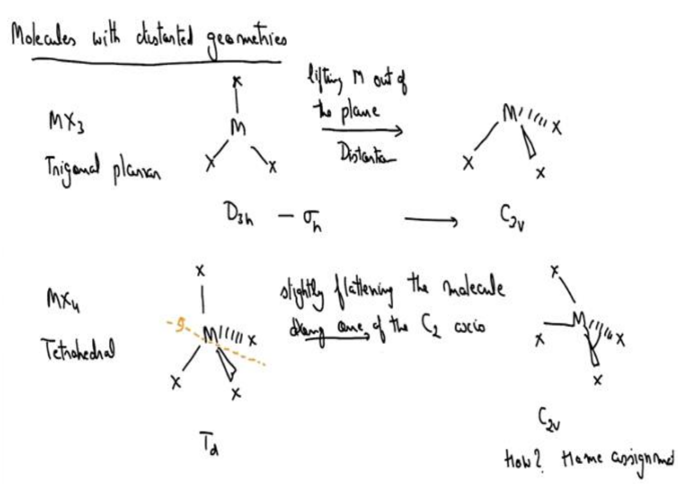

Let us now look at some molecules also. And let us see what happens if we distort these molecules. So, we will be looking at molecules with because regular geometry we all understand by now, but what happens if we distort these molecules how the point group changes with distorted geometries. So, when I say distorted geometries, we will just change the bond length of one particular bond hypothetically?

I mean, it can happen in real time also, depending on what kind of ligands are available and so on, so forth. So, here we will be doing only hypothetically, so you have an MX3 molecule, let us say it is the first molecule is trigonal planar. So trigonal planar is you have M, X, X, X. So, this one is simple D3h, so I am not going to work out this molecule I will just tell you how the distortion changes the point group now.

So, let us say the distortion is this is my distortion where, what I am doing is I am lifting M out of the plane. So, what happens if I lift M out of the plane of the board, so, then it basically becomes like an umbrella. So, you have X, X, X. So, top view still looks like this, but what you have done is you have lifted M out of the plane of the board. So, now from D3h, now you have gone to C3v. Later on we will see how these kinds of distortions are actually very important to understand.

But today we are just focusing on how a particular distortion changes the point group. So, you have from D3h you went to C3v because what you have done is you have basically killed, sigma-h in the process. So, I can say if I am removing sigma-h out of this, so, I will lead to a C3v kind of thing, the rest of the planes and all other symmetry elements are still present and it must follow the closure property of the group which it does follow. So, what you are left with is C3v.

So, let us do similar kind of distortions in different molecules and see, so, let us say if you now have MX4, which is originally tetrahedral. So, then, you know how to draw a tetrahedral molecule. So, you have X, X, X and this is a Td point tetrahedron. Now, what is the distortion here, distortion is so what question says slightly flattening the molecule along one of the C2, axis. So, what you are doing is, where is the C2 axis, let us draw the C2 axis here.

So, this is my C2 axis in the plane of the board, this will be reflecting on these 2 Xs and these 2 Xs. So now if I flatten this molecule along one of the C2 axis, how does it look, so, these 2 will not be flattened, because I am trying to flatten about this C 2 axis, so these 2 will not be affected. Or let us say these 2 will also be affected, let us do one by one. So, let us first distort only these 2 angles.

So, what I have is basically you have M, X, X and what you have is X, X. So, now, this angle is no more 109 degree 28 minutes, this angle is still the same as Tetrahedral angle. So, that would mean what will be my point. So now my point group will be C2v and how do I get C2v? Try to work it out yourself. Here, I am giving you the point group answer and I am asking you to find out all the elements and see if this is correct or not.

Similarly, if you compress this angle also, again you will end up getting a C2v point group. So, try to work it out and see this kind of distortion, how this kind of distortion, what all elements what else symmetry elements are killed in the process, when you do this distortion.

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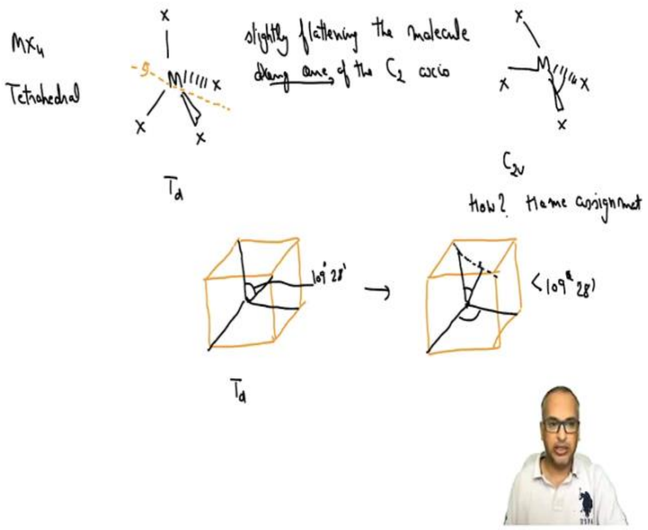

So, if you have difficult in understanding this distortion, maybe what we can do is we can draw this molecule inside a cube and do the same distortion. So, inside the cube, if you draw it will be a tetrahedron. You have center, one bond is going to this diagonal one bond to this vertex, this vertex, and the vertex. So, this gives you a tetrahedral. So, this is a Td geometry, now, the distortion actually takes it to a different one.

So, let us see what is the distortion here what we have done here is this is my center again. So, these 2 bonds are now compressed, let us say what we have done is we have compressed only these 2 bonds. So, instead of going to vertex now, they are falling on one of the face diagnols, this is how the distortion looks like. So, instead of all the way to the vertices, now, I am resting my bonds or my atoms at the, somewhere in between the face diagonal.

So, now, that means this angle which was initially 109 28 minutes degree 28 minutes, now, this is less than 190 degree 28 minutes, rest of the angles, angle is all the other angle is still the same, it will of course, affect other angles also. So, now, what all elements are killed in this process that you have to visualize? So, what do you have basically, what you have to do is you have to sit inside the cube yourself and see how the bonds are changing or how the elements are affected?

How many C4s or C3s or C2s are there initially when it is it was a tetrahedral and now what we are left with is only C2v, is that correct? Do we have more symmetry elements, do we have less symmetry elements so, try to work it out? So, I have given you an approach how to solve this problem, this kind of problems, but try to work it out yourself otherwise, we can always discuss during the interaction session.

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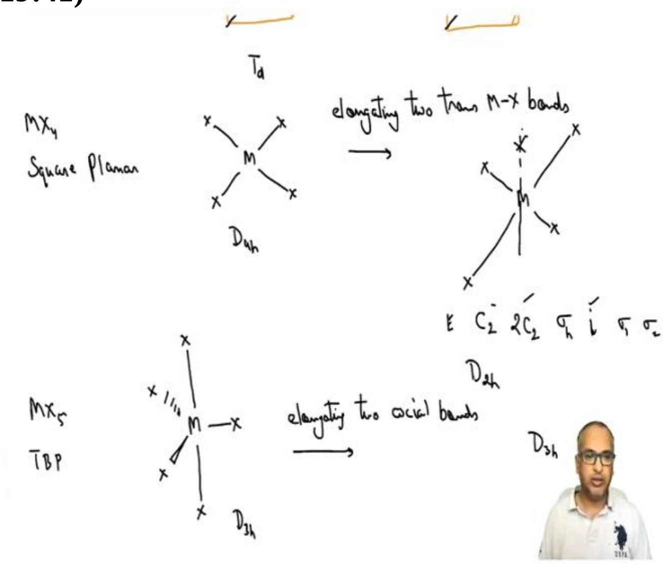

So, let us take more examples like this. So, this one is simple. So, you have MX4. Originally, the geometry is square planner. So that would mean or D4h point group. So, you have MX4 like PtCl4 for you have D4h again we are not going to discuss and now that distortion is elongating 2 trans MX bonds. So, that means, I have to elongate these 2 and these 2 are kept at same distance.

So, that would mean my molecule now looks like, so, I have done this distortion now, how this thing will change now, what do I left with so, I am left with so, first of all I have killed my C4. Now, there is no central C4 axis, principal axis is not reduced to C2, C2 which is coming out of the plane of the board perpendicular to this so, that these 2 are reflected and these 2 are reflected.

That is C2 and then you will also have C2s which will be so, these C2s are also killed now, you do not have this C2, this C2 is not there. So, what you have is this C2 and the C2. So, basically now, you have 2 C2s perpendicular to your original C2, that means it is a D2h point group. Other than that, you also have you are still left with sigma-h, you are still left with i. So, sigma h, and then you will have 1 sigma here, so, sigma 1, sigma 2. So, basically 3 sigmas are there.

So, this will be D2h kind of point group so, let us verify this let me look at the D2h connector table. So, the D2h should have E, 3 C2s which are perpendicular to each other. So, you have this i, and then 3 sigmas again if one is along xy another will be yz third will be zx which we have. So, that is correct. So, basically by elongating these 2 bonds from D4h we are going to lower symmetry point group we are going to D2h.

So, why did I say lower symmetry point 2 because here the order of the group is lower. So, now, let us look at more examples. So, you have MX5, which is trigonal bipyramidal what will be the point group here? So, let me draw the molecule. So, in this case equatorial bonds are of different length and axial bonds are of different length. So, this is a trigonal bipyramidal case, what will be the point group?

Point group is D3h here. And the distortion I am looking for is elongating 2 axial bonds. So, if I am elongating two axial bonds, they are anyways elongated. So, if I elongate it further or decrease the length of these MX bonds, it should not change anything. So, the point group remains as D3h. So, this is a simple case.

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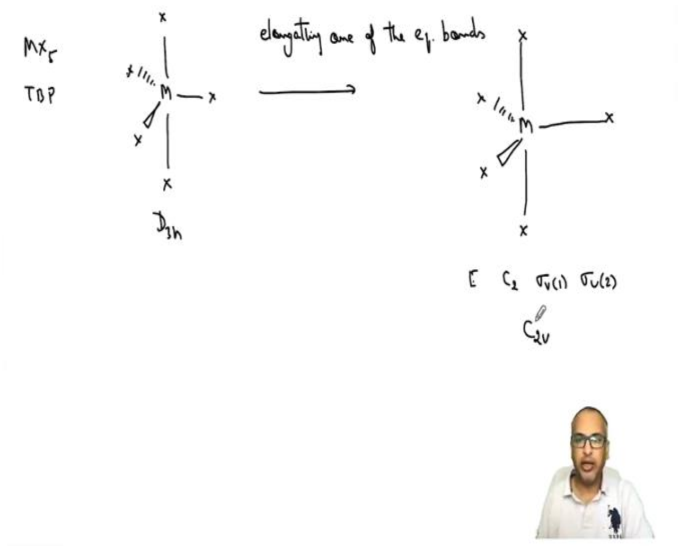

Now, let us look at more such trigonal bipyramidal cases, you have again you have MX5 trigonal bipyramidal, and the distortion now will be different. So, again this is D3h and the distortion is what we are doing is elongating one of the equatorial bonds. So, if we elongate one of the equatorial bonds, what do we get? And what are the symmetry elements that we are killing.

So, let us say this is elongated and now try to think that where are we now? So, this looks like water molecules. So, what you have got is E, C2. C2 is passing through this MX bond, sigma is again the plane of the one will be the plane of the board another is perpendicular to the plane of the board, both containing this elongated equatorial bond MX. So, you have sigma v 1 and sigma v 2. So, point group will be C2v. So, again from D3h we have gone down to C2v, gone down in order of the group.

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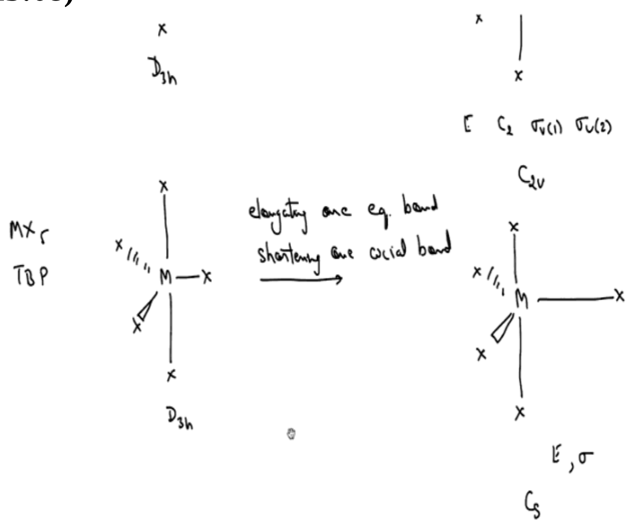

Let us look at more examples, 2 more examples. So, we have again we have MX 5 and we are starting geometry is trigonal bipyramidal, so and the distortion. So, this is D3h, distortion here is while we are elongating one of the equatorial bonds, 1 equatorial bond and simultaneously, we are shortening 1 axial bond. So, let us see how it works out so, you have MX elongated these 2 are not changed, this one is reduced in length, this one is still the same now, what do you think will be the point group? So, what do you have?

So, now, if we try to put a C2 axis here along this MX bond, I do not have any C2 axis because although these 2 will be exchanged, but these 2 axes will not be exchanged, because their bond lengths are different. What about sigma there is no sigma in the plane of the board, but there is 1 sigma which will contain the 2 axial and 1 equatorial and this M atom. So, these 2 will be reflected.

So, we have E and we have sigma any other symmetry element, we do not have any other symmetry element, no C3 axis here, because these 3 will not be rotated. So, the point group now is Cs point group. E and sigma that is all. So, that is also easy, but see now, when we are doing any kind of distortion, what you have to keep in mind is that what are the symmetry elements originally present?

And by doing this process out of those symmetry elements, what elements got killed because of distortion? So, if you can think in those lines, you should be able to find an answer very quickly.

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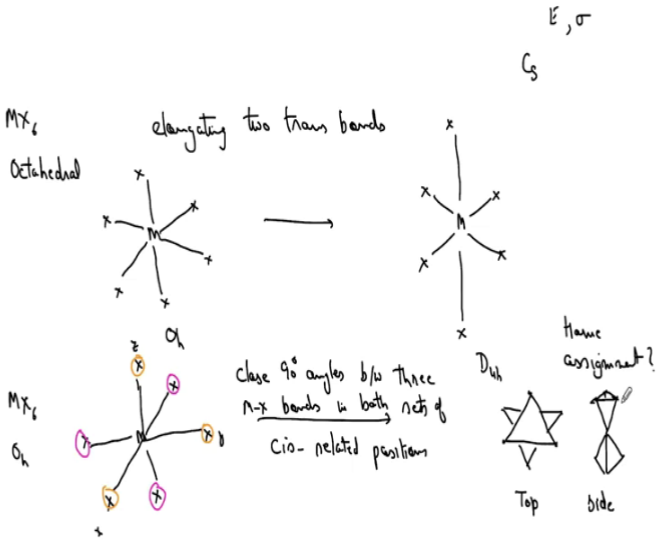

Let us do one more example. And then we can stop. So, let us say MX6 octahedral case. So, let us say, let me do 1 example and one I will give for home assignment, so elongating 2 trans bonds, this is a simple one. Let us do both. So, how does it look? So, you have M, all the bonds are of same length. So, they are equally spaced out. Now, this is Oh point. This is the distortion elongated 2 transforms which can be anything maybe you can take top and bottom or you can take this one, this one anything will give you the same result.

So, let us say elongate these 2 bonds. So, what happens now, what we have done is we have killed a lot of elements from Oh we have gone down to D4h. Now how does it work? So, try to again find out the missing elements, what all elements are killed in the process and hence the this becomes a case like PtCl4, so D4h you all know by now that what all molecules would look like D4h so.

So, this looks like a PtCl4 kind of molecule, let us do one last example. This is a slightly tricky one. So, I want to cover this, Octahedral again. Now, here let me first draw the write the distortion. So, it says close 90 degree angles between 3 MX bonds in both sets of cis-related positions. So, it is a little tricky to understand what the question is asking, cis-related positions.

So, if we try to draw a coordinate system and put the molecule on to this, so, you have basically M sitting here X, X, X going along the coordinates, which is x, y, z and the other 3 are sitting like this. So, now, if you consider this X, let me circle this, this X, this X and this X, this they are one set of cis-related positions, the other 3 are other, so, let me draw it with a different colour.

So, the pink set is a second set. Now, if you notice that the angle between x axis y axis and z axis is 90, 90, 90. So, now, they are saying that close that angle so it is like an umbrella which is opening up and then you are closing down x, y and z axis to an angle less than 90 degrees. So, x, y, z are no longer perpendicular to each other, they form like a cone? So, if I am looking from the top, it looks something like this, something like a star.

That is how octahedral in general would look like, but now, these 3 vertices are not meeting at a point where those axes are forming 90-degree angles. So, if I look from the side, it looks something like this, it looks like a cone shaped thing. So, this is the top of the star and these are the bonds and is the third bond is that the back and the other one will be so you have one bond in the front.

So, this is how it looks from the side. So, this is the top view and this is the side view. So, I hope it is easy to see now that what all elements got killed. So, I have already drawn this molecule for you. So, I would give you as a home assignment. So, try to work it out. What is the point about this molecule? So, try to see this the most complicated one, but if you cannot find it, will again discuss during interaction session.

But if you can find it well and good, so try to work out what all symmetry elements are killed in the process and what is the point group of the final? So, I think that is also we have discussed a lot of examples today. So, keep practicing. So, this course requires a lot of practice. So, if you cannot figure out the point group of a molecule, the rest of the course will be very, very difficult. So, I would suggest you to practice a lot of molecules and then we can cover the rest of the topics very easily. So that is all for today. Thank you.