Mathematics for Chemistry
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Lecture - 31

In the last lecture, we looked at the various groups that are formed, when you have multiple C n axis, where n is greater than 2 and this pretty much will allow us, to classify all the molecules into various groups. So, based on which operations are present, we can classify molecules into various groups. Now, if you look at the character table of any molecule, what you see in this, are not individual symmetry operations, not the individual operations in the group but what you see are the classes of operations.

And so what you are going to do in the next few minutes is, to look at the classes of operations and use the standard notation, which is now common in writing various groups. So, finally we will go to something called the character table and in the character table, what appears are not individual operations, but actually classes, classes of operations. So, we will just spend a few minutes discussing how to get these classes of operations and then we will look at the notation that is used for character tables.

So, we have already discussed in some detail, the various classes of symmetry operations, we said that two symmetry operations are in the same class, if they are related to each other through a similarity transformation. Another way of stating this is, we will see this right now and we will look at it through an example.

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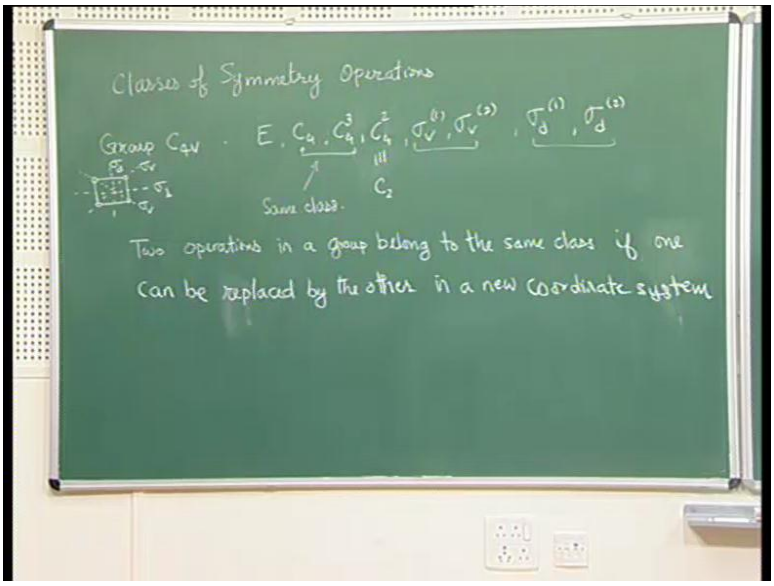

So, let us take the group C 4 v, so C 4 v is a group and the various operations of this group, you can work this out. These are E the identity, there is a C 4 axis and C 4 generates three more operations C 4, C 4 2 and C 4 3, I deliberately wrote it in this order. C 4 2 is identical to C 2, C 4 2 is rotation by 180 degrees, which is same as C 2 and then there are 4 sigma v planes, two of them are refer to as vertical planes and two of them are refer to as dihedral planes.

So, you can think of a planar molecule, if you think of a molecule that is planar then the C 4 axis would be one, that passes through this and you would have these two as a sigma v axis and these two being so this is sigma v, sigma v and these two are sigma d's. So, we have these sigma v's and sigma d's, C 4 v it is not actually for planar molecules but to illustrate the difference between sigma v and sigma d I am using this geometry.

Now, what you will show if you work out the group multiplication table, you can show that, C 4 and C 4 3 are in the same class, sigma v 1 and sigma 2 or sigma d 1 and sigma 2 are also in the same class, C 2 is in a separate class, E is always in a class of its own so these are the various classes. Now, we will just look at, we will take the example of C 4 and C 4 3 and we will show something that is, you know in a sense, we will explore further the relation of them being in the same class.

So, we had stated this way of writing classes, as defining classes, as two operations in a group belong to the same class, if one can be replaced by the other in a new coordinate system. So, essentially, what we mean is that, in one coordinate system, you will have C 4, one operation look like C 4 and the other look like C 4 cube. If you look in another coordinate system, first operation will look like C 4 3 and the second operation will look like C 4 but that is not all, this is not all.

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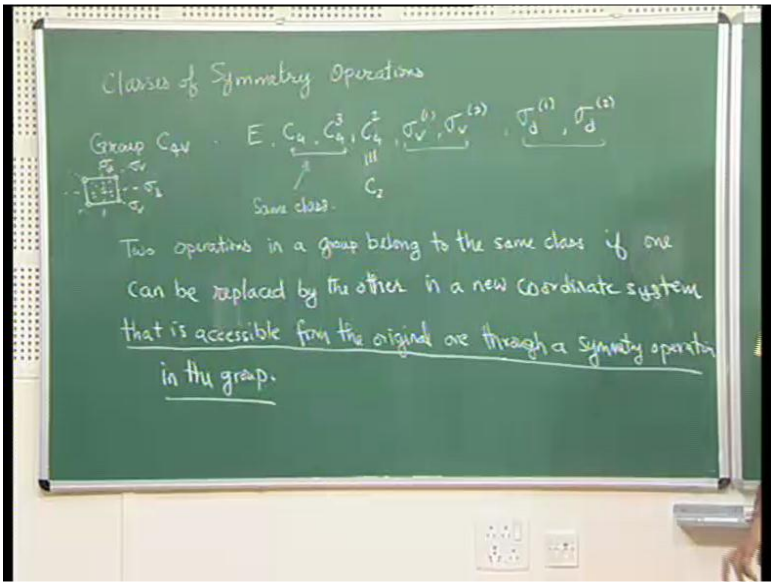

So, in a new coordinate system and this new coordinate system should be accessible from the first, from the original one through a symmetry operation in the group so this part is very important. It is very important that, the two elements will be in the same class, only if they can be replaced by the other in a new coordinate system. So, in one coordinate system, C 4 looks like one transformation and C 4 looks like something else and that something else, looks like C 4 in the other coordinate system. But, then these two coordinate systems should be accessible from through a symmetry transformation, through a transformation that is actually a symmetry operation in the group and we will look at this example.

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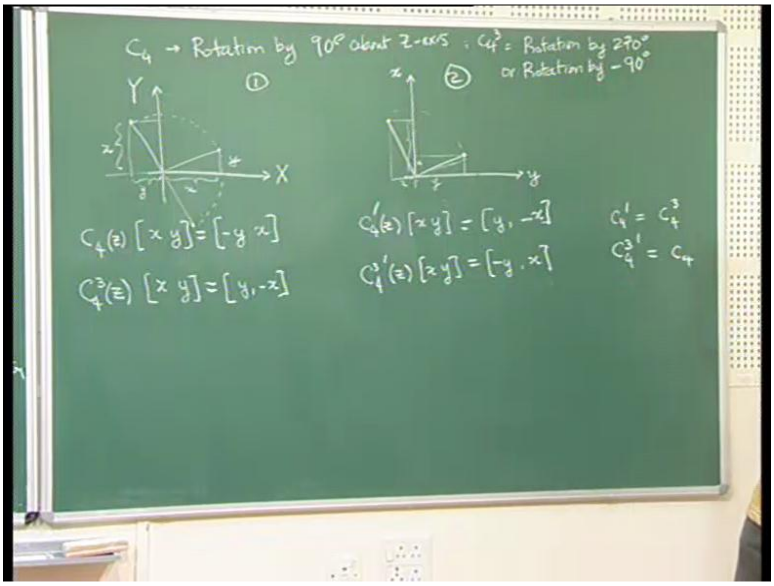

So, let us look at so C 4 is same as rotation by 90 degrees, so C 4, you can think of as rotation by 90 degree about the z axis. So, if you think of it that way then if you have a coordinate system, I will call this coordinate system 1 where, you have X and your Y axis. Now, if I take a point with coordinates x and y, and I operate it by C 4 so C 4 is rotation by 90 degrees and if you rotate by 90 degrees then this point will come to this point.

Now, the x coordinate of this point is same as y but the x coordinate has changed sign so this distance is y, this distance is x. So when you operate C 4 about z axis on an arbitrary point x y, you get a point so the new x coordinate is minus y and the new y coordinate is x so this new point has coordinates minus y and x. Now, if I rotate by 270 degrees so C 4 cube equal to rotation by 270 degrees or rotation by minus 90 degrees so you can either rotate by 270 degrees or you can rotate by minus 90 degrees.

So, if I do C 4 cube on z so then it takes a point x y now, we can show what will happen so if I rotate by minus 90 degrees, I will end up exactly here so the point will be exactly y, minus x. So, it will be exactly opposite of this that is, y minus x now suppose, I do the same thing in a slightly different coordinate system where, let us say, this was my y and this is was my x. If I had y and x define this way then you can see that, C 4 will take this point here.

You can show that, if you had a point with x coordinate as x and y coordinate as, this is the y coordinate that is, y and let me call this coordinate system 2. So, in coordinate system 2, I will call it C 4 prime, just to distinguish it from that so in this coordinate system, the point x y gets map to y, minus x. So, you can see that, the x coordinate of this new point is same as y so this is y and the y coordinate of this new point, which is this distance that is, minus x.

Similarly, C 4 cube prime of z of x y, this is equal to minus y, x so here, we see the same C 4 operation, in this coordinate system it takes x y to minus y, x whereas, in this coordinate x y to y and minus x. Similarly, C 4 cube in this coordinate system takes x y to y, minus x and in this coordinate system, it takes it to minus y, x. So, you can see that, C 4 and C 3 are interchange, the effect of these two operations is interchanged in this new coordinate system.

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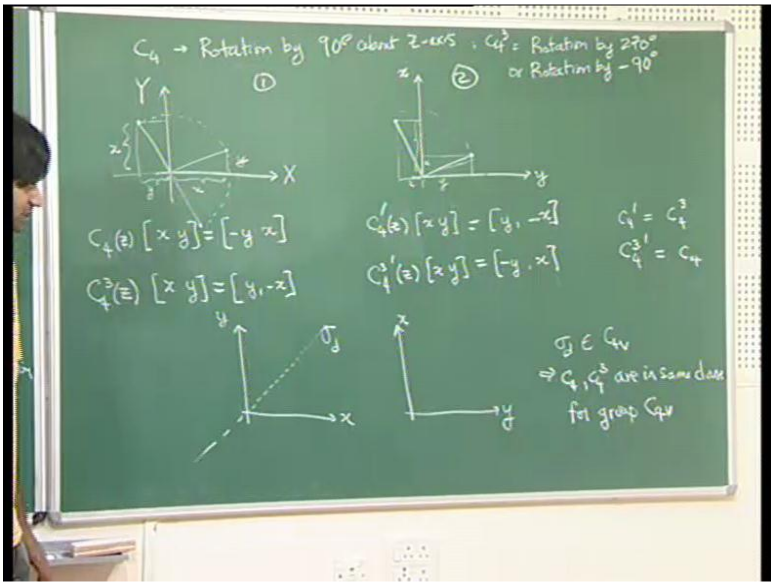

So, in other words, C 4 prime is equal to C 4 cube and C 4 3 prime is equal to C 4 so in this primed coordinate system, C 4 and C 4 cube have the opposite effect on the same point. Thus, we found a new coordinate system, in which these two operations can be switched now, that is not all, you need these two coordinate systems to be related through a similarity transformation, through a symmetry operation.

So, what is the symmetry operation, that takes this coordinate system on to this so in other words, what is the symmetry operation, that takes y from here to here and take x from here to here. And you can see it very easily so if you had this as your y and this is as your x now, you want a symmetry operation, that leads to x here and y here and it is very easy to see, that the operation, that you have has to be a reflection about this.

So, if you reflect about this axis then this becomes your x axis so if you imagine there is a mirror here, that reflects it so x will come here, y will come here and you will have something like this. Now, this reflection corresponds to a sigma d operation, either sigma d 1 or sigma d2 depending on, how exactly you define the various axis. So, sigma d takes this coordinate system 1 to coordinate system 2 and in these two coordinate systems, these two operations are interchanged.

So, this implies, since sigma d is contained in C 4, sigma d is one of these sigma d's is contained in C 4 v. So, you have an operation sigma d, which is contained in the group, which takes, which transforms this coordinate system 1 to coordinate system 2 such that, the C 4 and C 4 3 get interchanged in these two coordinate systems. And that is why, you say C 4 and C 4 3 are in the same class so this implies C 4, C 4 3 are in same class for group C 4 v.

So, they are in the same class, only if you have C 4 v group, only if you have this additional sigma d operation in the group, that takes one to another. So, for example, if you had the group of pure rotations now, a group of pure rotations like C 4, C 4 would be a group of pure rotations where, these operations would not be there. So, if you had a group of pure rotations then C 4 and C 4 3 are not in the same class, C 4 and C 4 3 turn out to be not in the same class for this group of pure rotations.

In fact, if you have a group of pure rotations then each of these elements is in a class of its own so now, this way of understanding classes of symmetry operations is extremely useful. Because, this seems to suggest to you that, there is something very similar about C 4 and C 4 3, there is something that is, I mean they look like the same operation. So, these two operations are basically the same operation, it is just like, you look at it in a different coordinate system then this will look like this and this will look like this.

So, these two are essentially the same operation, one is just rotation by 90 degrees one way, other is rotation by 90 degrees the other way. But, if you had a coordinate system where, one way look like the other then these two operations would get interchanged. So, there is something that is very characteristics of these symmetry operations and it is that operations, that are in the same class. So, two operations in the same class, they are related to each other through the simple coordinate transformation.

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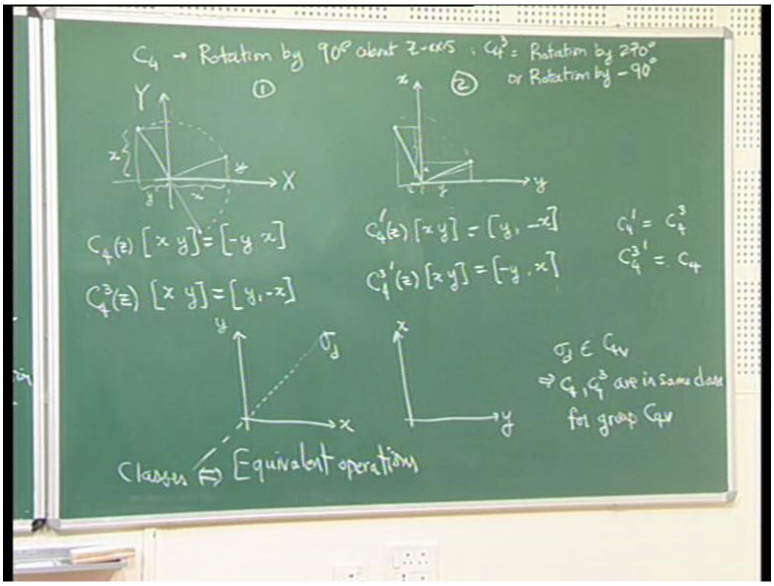

In a sense, what we said is that, the classes so if two operations are in one class then those two operations are essentially equivalent operations. So, two operations in a class are basically equivalent operations and so this C 4 and C 3, these two turn out to be in one class. Similarly, you can show that, sigma v 1, sigma v 2 turn out to be in the same class similarly, sigma d 1 and sigma d 2 will turn out to be in the same class, sigma 2 is in a class of it is own, E is in a class of it is own.

So, since two operations belonging to the same class are essentially equivalent operations, it make sense to them together and that is what, is done typically when we write the character table of groups. So, I will just do it right here, when we write the character table of the of the group, we divide the elements of the group into classes.

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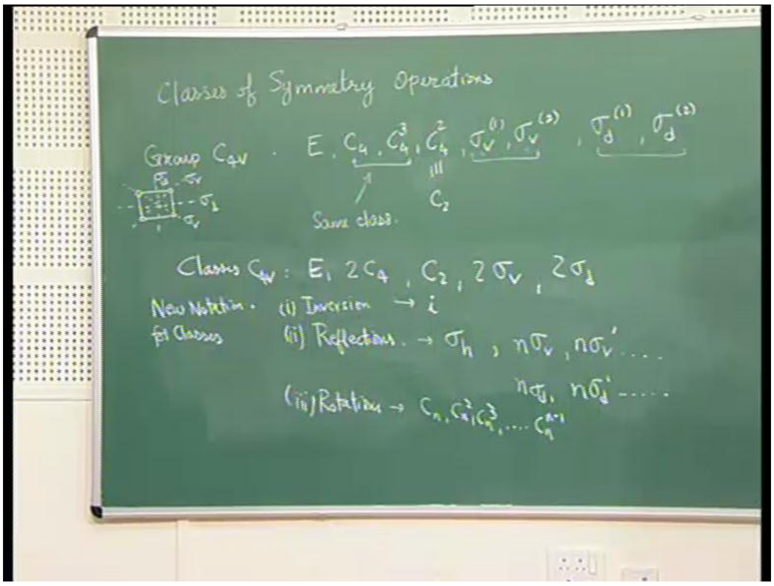

So, when we list the various operations of this group so we will write it in this form, E now, there are two operations in the same class as C 4 so we write it as 2 C 4 then there is C 4 2, which is same as C 2. So, we just write C 2, this is 2 sigma v and 2 sigma d so we write them in classes so these are various classes. So, these are the various classes in C 4 v and this is one way to list all the operations.

So, the way to read this is, there is the identity operation then there are two equivalent C 4 operations, there is one C 2 operation, there are two equivalent sigma v’s and two equivalent sigma d ‘s. Now, this notation in terms of classes is, what is used in most of the character tables so let us just try to write down the rules for writing such notations so this is a new notation and let us write the rules for this.

So, the rules are, for each operation you can write the rules so for inversion represent by i so the class is represented by i, so new notation this is for classes. So, if you have a centre of inversion, you can have only one centre of inversion in a molecule and if you have that then you just represent it by i, i is in a class of it is own so you just call that class i. Second is reflections so if you had a sigma h, sigma h is always in a class of it is own so we just call it sigma h so sigma h will be in a class of it is own.

Now, if you have a sigma v’s then you separate them into classes so sigma v’s and sigma d’s are separated into classes. And you can have n sigma v’s in one class, you can also have cases where, sigma v’s divide themselves into various classes. So, some sigma v’s are in one class, you could have another sigma v prime in another class and so on. And then you could have sigma d’s and this, which class you call sigma v and which class you call sigma v prime is quite arbitrary.

So, good example is here, here you had 2 sigma v and you had 2 sigma d now, you could have more sigma v planes, which happen to be in the same class but not the same class, as these two then you would list them as n sigma v prime. The third is rotations and here, we have to consider two cases, if you had pure rotations suppose, you had C n, C n 2, C n 3, C n n minus 1, so these are the various operations. Now, if each of these was in a class of it is own then you would list the classes in this way so if they were in the class of their own, you would list it this way. Sometimes what happens is, as we saw in this case, because of the additional symmetries, some of the rotations fall in the same class.

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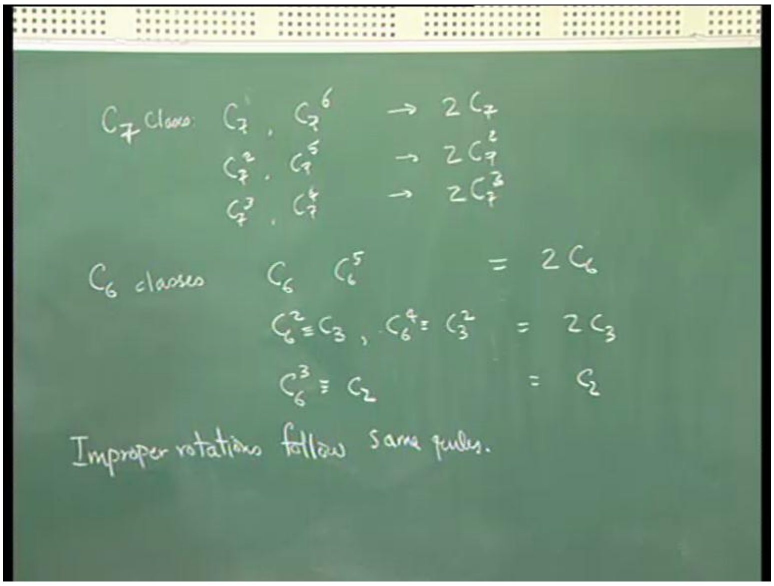

So, for example, you could have had suppose, you had C 7, you could have a case when C 7 has C 7 1 or C 7, C 7 6, C 7 2, C 7 5, C 7 3, C 7 4. So, you could have this example where, in C 7, if you had 7 sigma v planes then these two would be in the same class, sigma C 7 is rotation by 2 pi by 7, C 7 6 is rotation by minus 2 pi by 7. And if you had a sigma d just like in that case then these two would be operations in the same class.

So, then this class you call is as 2 C 7, this class we will call it as 2 C 7 2, this class we will call it as 2 C 7 3 and so on, and you can do this for other operations. So, when these two are in the same class so if your classes now, these two will be in the same class, only if there is a sigma operation, that helps you transform coordinate so that, one looks like the other.

Now, for example, if you had C 6, you could have had C 6, C 6 5, these two could be in the same class, C 6 2, which is equivalent to C 3 and C 6 4, which is equivalent to C 3 2. Then you could have had C 6 3, which is equivalent to C 2 so these two with the classes called 2 C 6, this it is called 2 c 3 and this it is called C 2, you have two classes containing two elements and one class containing one element.

So, this is the way, you list the various operations, you break them into classes and then you use this notation for the classes and just as we did for the proper rotations, you could do the same for improper rotations. So, improper rotations follow same notation, follow same rules so instead of C's, you have S so if you had an S 6, S 6 and S 6 5 could be in one class, S 6 2 and S 6 4, which is you know, they would be in the same class and so on. Now, that we have seen, how to separate the various operations into classes, we can now go ahead and give the procedure for classifying various molecule into groups.

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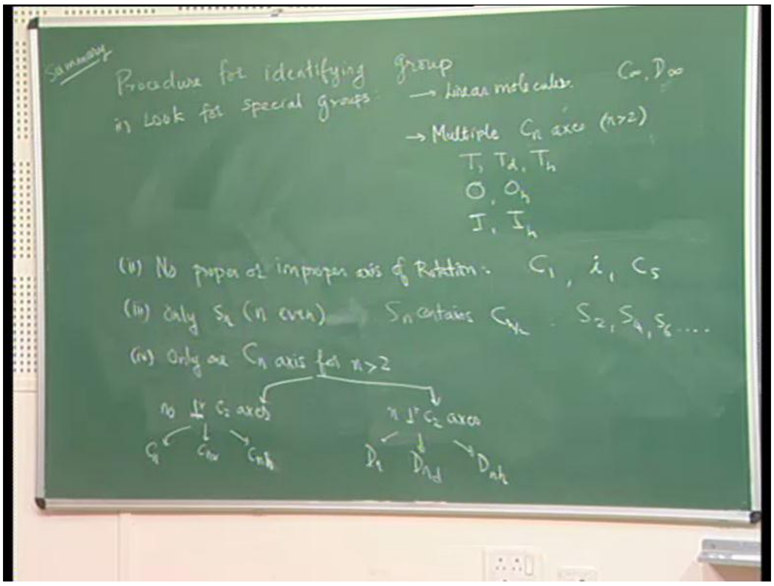

So, this is the procedure for identifying group so the idea is, have a molecule, you have all the symmetries suppose, you know all the symmetries, how do you identify, which group utilize them and this is the summary of, what we have been talking about in the last 2 or 3 lectures so this is the summary. So, how do you go about identifying the group, in which the molecule should lie so the first thing, look for special groups.

So, the special groups, I mean linear molecules and molecules with multiple C n axis where, n greater than 2. So, first you check, whether your molecule is linear, if your molecule is linear then the group will be C infinity or D infinity. So, if our molecule is not linear, you will see whether your molecule has multiple C n axis where, n is greater than 2 and this is… So, if it has then it has to be one of the seven groups, T, T d, T h, O, O h, I, I h so it has to be one of these seven groups.

So, if it has multiple C n axis where, n is greater than 2, it has be one of these seven groups so first you check, whether it falls in one of these special groups, if not then you look for molecules, that have no proper or improper axis of rotation. So, if a molecule does not have any proper or improper axis of rotation, then it will be either a totally a symmetric molecule that is, C 1 or it can be a molecule with a centre of inversion, or it can be a C s, that just has a mirror planes.

Then, the third so first you look for special groups, that are linear molecules or molecules with multiple C n axis, then you look for molecules, that do not have any proper or improper axis of rotation. Then you look for molecules at only have S n and obviously, n has to be n even so only S n where, n is even. So, if S n is even so S n 2 is same as C n by 2 so it has only S n axis where, n is even remember, S n contains C n by 2.

So, if it only contains S n then the name nomenclatures like S 2, S 4, S 6, etcetera so it has to be one of those groups then the fourth one is, only one C n axis for n greater than 2. So, when you have only one C n axis for n greater than 2 then there are two cases you can have, you can have one case when there is so the two cases the first case is, no perpendicular C 2 axis so we do not have any C 2 axis, that is perpendicular to this C n axis.

Now, you should recall that, if you had a C 2 axis that was perpendicular then you would have n other C 2 axis. So, in this case, if you have no perpendicular C 2 axis then you can have either c n where, you have no sigmas or you can have c n v or you can have c n d's. So, if you have a vertical plane of reflection or dihedral plane of reflection, it will be either C n or C n v or C n d sorry or C n h.

So, if you had a horizontal plane of symmetry then it would be C n h now, the other case is, if we have perpendicular, n perpendicular C 2 axis so n C 2 axis that are perpendicular to the C n axis then you can have three cases. So, the corresponding cases will be D n and D n d or D n h so in this case, it will be a group of, the name of the group will be either D n, D n d or D n h so this little chart will help you take.

Look at the various operations, various symmetry operations of a molecule and identify, and assign it the appropriate group. So, this whole procedure is a summary of, what we have been discussing so far, once you have all the operations then you can go ahead and you can tell, which the group molecule lies in. So, let us do an example of this, this is the Allene molecule, I will take an example.

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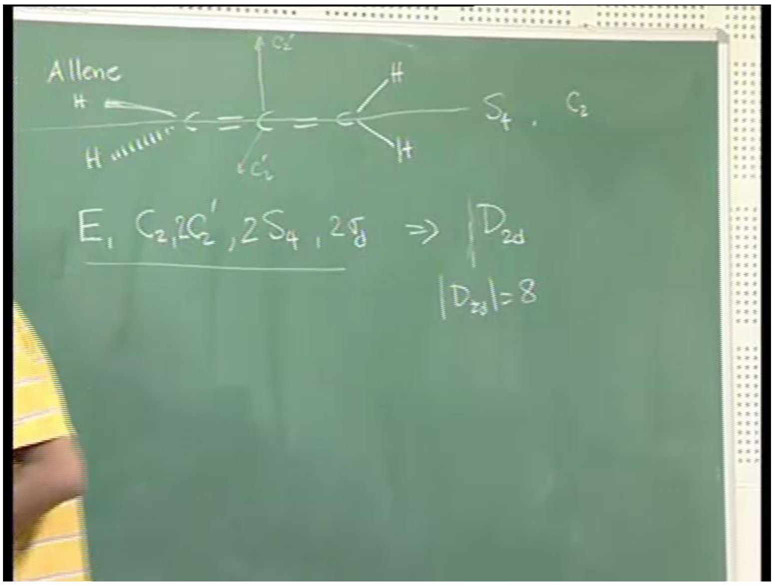

So, Allene molecule has C, it has C and now, this has 2 hydrogens and this has 2 hydrogens. Now, these two hydrogens would be, if these two are in the plane of the paper then these two would be perpendicular to the plane of the paper so they will be one going in and one coming out. So, that is what the Allene molecule will look like so let us list all the symmetry operations of this molecule.

Now, you can show that, this axis is an axis of rotation and this axis is an S 4 axis, it is also a C 2 axis, so this is an S 4, it is also a C 2 axis in fact, S 4 square, S 4 itself generates C 2. Because, if you operate S 4 twice, you will get a C 2 operation but notice that, there is no sigma h in this molecule, there is no sigma h and there is no C 4 but there is an S 4.

So, also you can see that, since these two hydrogens are equivalent so if you can have a C 2 axis here and a C 2 axis here, so these two are also C 2 axis. So, these two C 2 axis will turn out to be in the same class. So, we will call them 2 C 2 prime then this has C 2, which is generated by this S 4, that will be in it is class of it is own and then there will be S 4 and S 4 cube so that is 2 S 4.

So, these are the various operations and then there should be a dihedral plane so there should be two dihedral planes, one is perpendicular to the board and one is in the plane of the board. So, there will be two sigma d's and these two are equivalent, so you can list the various classes in this way and so there are 2 4 6 7 8, 8 operations. So, if you follow this classification scheme, you have 1 C n axis, that is 1 S 4 axis, you have 1 S 4 axis and you have no perpendicular C 2 axis.

So, this you can show that, this is in D 2 d so it is d 2 because this is the C 2 axis and it is C 2 and there is no perpendicular C 2 axis. So, these set of operations, this group is called D 2 d, the size of this group is order of D 2 d equal to 8. So, next, what we want to look at, is the representations of these groups, so let us look at some examples of, how we would identify the symmetry group of various molecules, based on their structure.

Now, the examples I will take, will be illustrative of all the rules, that we have discussed so far so we looked at the Allene molecule. Now, we will look at two some other examples and you should actually go back and try to verify some of the things that we are saying here.

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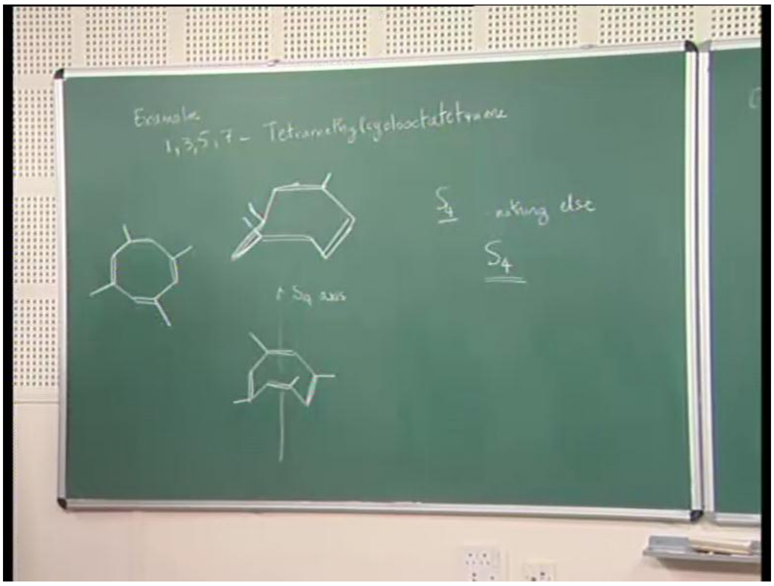

So, let us take the case of 1 3 5 7 tetra methyl cyclooctatetraene so this is basically a molecule, that looks like this. So, it has 1 2 3 4 5 6 7 8, so it is a cycloocta and there are 4 double bonds, tetraene so and this 1 3 5 7, so this is the tetraene and there are 4 methyl groups. So, this is cyclooctatratene and there are 4 methyl groups located at 1 3 5 and 7 so you can put 1 methyl group here at alternate so there are 4 methyl groups, this is the molecular structure of this molecule.

Now, the three dimensional shape of this molecule turns out to be a little complicated but you can work it out. So, basically what happens is, you imagine that four of these three or you can imagine this way that, three of these form a sort of structure like this, there are three more that form a similar structure on that side. So, these 4 carbon atoms, 1 2 3 4 and 3 bonds, they form a structure like this, there is another parallel structure like this, you should actually imagine, it being directly behind this and these two are joint at this through a bond between these two.

So, this is the structure and you can see that, there are the symmetries of such a molecule will be in general little hard to determine and you have to really know, which direction the methyl groups point and so on. Now, this is a double bond so each of these are double bonds so if you know that, these are double bonds then you can immediately identify a few things, we will write this out here.

So, you have a methyl groups so the methyl group comes this way and you have this coming this way, you have a hydrogen here. Now, directly behind this in the plane of the board, you have another such groups. So, I will show it in front so it will be something like this. So, you have something like this and in this case now, the methyl group will be here so just imagine these two structures and now imagine that, you connect these two.

So, if I connect these two with a double bond, this is basically my cyclooctatetraene and then if I put methyl groups here and another methyl group here. Now, what you notice is that, because of these methyl groups, a lot of the rotation symmetries will be destroyed. What you also notice is that, if you imagine an axis, that passes right in between this so something like this. So, just this axis is an S 4 axis, it is S 4 because if you rotate it once then I mean you can see it from here.

If you rotate once then basically this double bond will come here and then you reflect it about a perpendicular plane, so then this double bond will go to the, it will come here and that will be completely symmetric with the original figure. So, this has an S 4 symmetry about it because you can see that by looking at this structure, so you imagine that, you rotate it once, then if you rotate it by 90 degrees. Then this will face sideways. So then what has happened is that they are double bonds or they turn appear in the opposite places.

So, when you reflect it then you will find that the double bonds appear in the right place and the methyls are pointing in the right directions. So, this is an S 4 axis now, because of these methyl groups, all the reflection symmetries are destroyed. Because, when you reflect about various planes then the methyl groups will start pointing different directions.

And so those reflection symmetries are destroyed because of, this methyl groups also, the methyl groups will also destroy any C 2 axis, that could have been present. So, this has S 4 and nothing else so it has only an S 4 and nothing else so the point group for this molecule is S 4. This is the rule you remember, if a molecule has S 4 group and nothing else, if it has S 4 group and nothing else then the point group of the molecule is S 4. So, it has an S 4 operation and nothing else, only in that case, it has a point group S 4.

If it has S 4 plus other operations, then it will not be an S 4 anymore, so an example of that is suppose, you just take cyclooctatetraene, which is same molecule without these methyl groups, the same as that molecule without the methyl groups.

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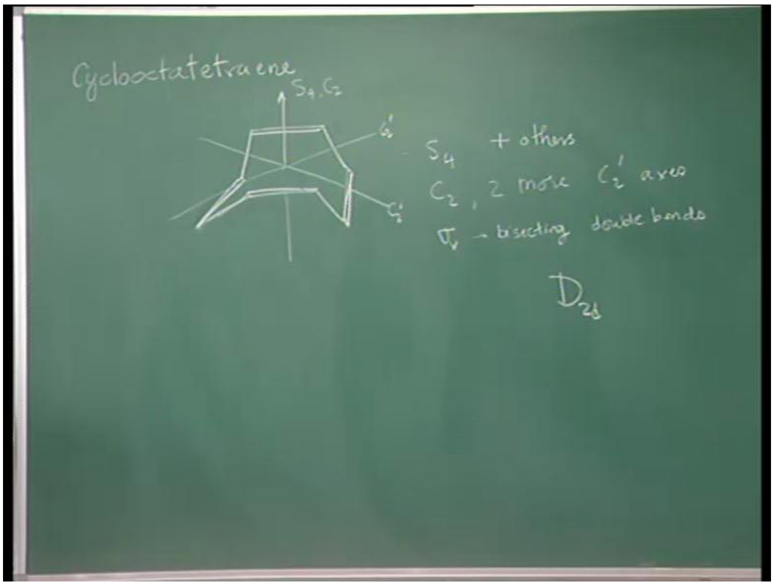

Now, what happens is, when you do not have these methyl groups, you have additional symmetries and you can see some of them. You can see that, you have 2 perpendicular C 2 axis in addition, this S 4 axis is also a C 2 axis, S 4 axis also becomes a C 2 axis because you rotate by 180 degrees, these double bond will go exactly here.

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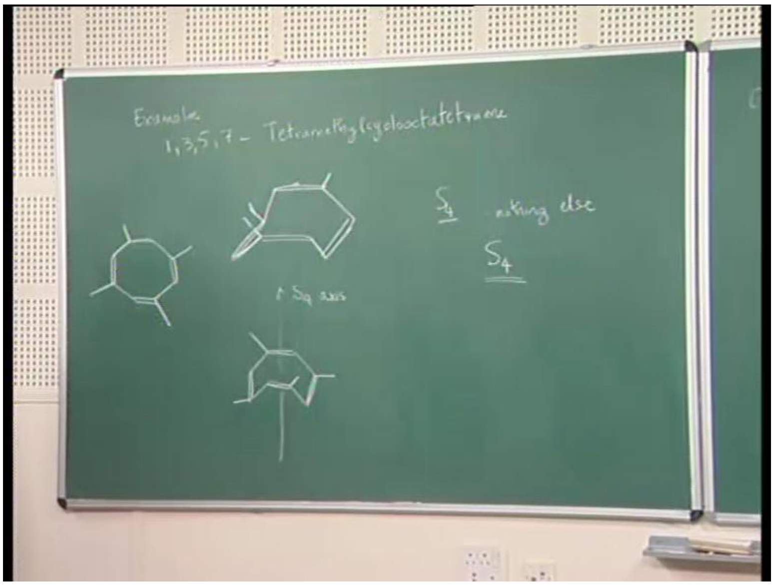

When you had the methyl groups, you rotate by 180 degrees, the problem was that, these methyl groups would not point in the right directions. So, that was the reason it was not for example, if you do a C 2 operation on this then you can see that, this will cause these methyl groups to point at different directions. So, if you do not have methyl groups then this has this S 4 axis, also a C 2 axis in addition, you have these two perpendicular C 2 axis, we call them C 2 primes.

And these are perpendicular to this S 4 axis and then you also have sigma v's, these bisect the double bonds. So, if we imagine a plane that passes through the centre of both these double bonds, that would be a reflection plane. So, if you reflect about this then this atom would come here, this atom would come here, this atom would come here, this atom would come here.

And then similarly, the other atoms should get reflected on this side, again that was the symmetry that was absent in the molecule with the methyl groups. So, the presence of the methyl groups again destroyed that reflection symmetry, that you have. So, now, since this has more than an S 4 operation, it also has other operations so therefore, you cannot say that, the point group is S 4.

Now, point group is determined by the C n axis, now the C 2 and you have sigma v so C 2 plus sigma v, that implies that, it should be D 2 d. So, the point group of cyclooctatetraene is D 2 d whereas, that of tetra methyl cyclooctatetraene is S 4. So, this is an example of illustration of the rules, I will show you one more well known example but again it is important that, you go back and verify each of these rules.

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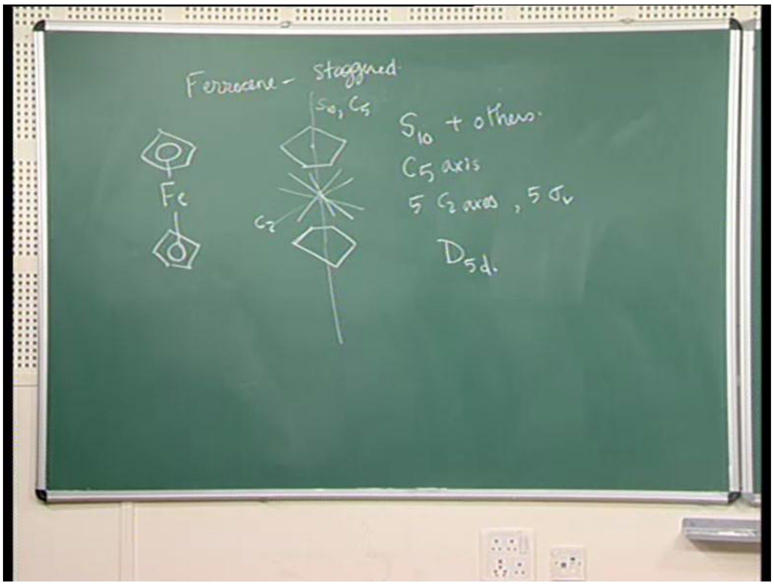

Now, let us look at the staggered configuration of ferrocene now, ferrocene if you remember the structure was something like this. So, this was your ferrocene structure and in the staggered configuration, these two pentagons are not exactly aligned. So, the way you would show it is that, you would show one pentagon in one direction and the other pentagon in the opposite direction so it show something like this.

So, these and you have this now, when these two pentagons are essentially planes, they are perpendicular to the plane of the board. So, you have a pentagonal structure there and another pentagon, that is staggered from this original pentagon. So, now, what are the various symmetry operations now, since we are staggered, first thing you notice is that, let us see there should be a S 10 operation.

So, there is an improper axis S 10 where, you rotate, you can imagine at this way so this axis is an S 10 axis so if you rotate it by 2 pi by 10 then this triangle will come right here. This bond will end up here and when you reflect it, it will get reflected on to this so it is an S 10 axis. So, this is a S 10 axis but there are other axis also, first thing is that, this is a C 5 axis, this is also a C 5 axis so S 5, S 10 plus others.

Now, this is a C 5 axis and what else can you say, what else is there so you can see that, there is a C 5 axis, 5 C 2 axis. So, there are 5 C 2 axis, that are sort of, I mean you should think of in this direction so there are 5 of these C 2 axis. So, if you have 1 C 2 axis, there have to be 4 other C 2 axis and then you can easily show that, there are 5 C 2 axis in this plane.

So, these are perpendicular to the plane of the board and they will be in various directions and there are 5 sigma v. Now, since it has in addition to S 10, it has C 5 so the nomenclature is dominated by C 5 so this is C 5 plus 5 sigma v so it is D 5 d so this is ferrocene staggered. Now, what about the eclipsed confirmation, what about ferrocene eclipsed.

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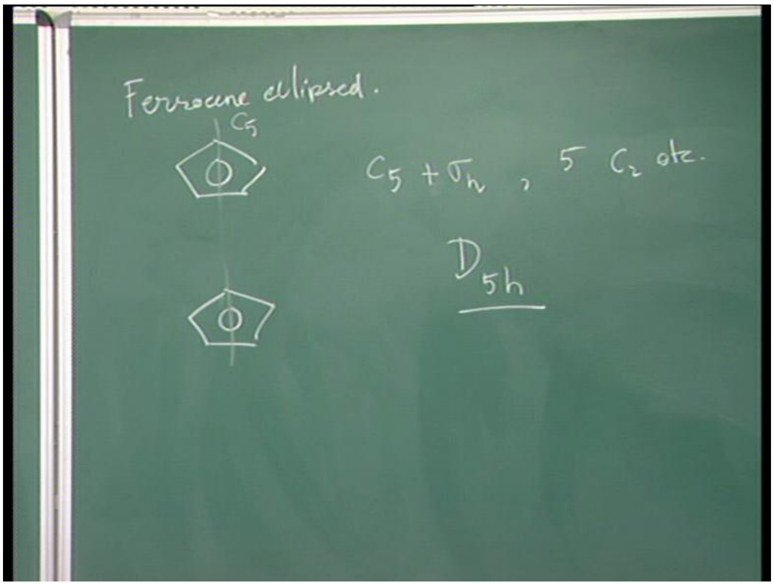

Now, in the eclipse confirmation, you have essentially something like this so these two are in the same direction so the two pentagons are both pointing the same direction. So, now, this is C 5 axis so you have C 5, now this plane is a plane of symmetry now, so this is a reflection plane. So, there is a sigma h so now, the nomenclature of the group will be dominated by this C 5 and it has sigma h, it has the vertical planes, as before it has various vertical planes sigma v, C 2, etcetera so this is D 5 h.

The presence of sigma h, it tells you that, it is D 5 h, sigma h, C 5, 5 C 2 and sigma h so this is D five by h. So, what we have seen is that, you know just the same molecule it looks like, just slightly different confirmations and they belong to completely different symmetry groups. If you have take something in between then you will get a different group for that, so we will get something in between these two and you cannot exactly say, what this is?

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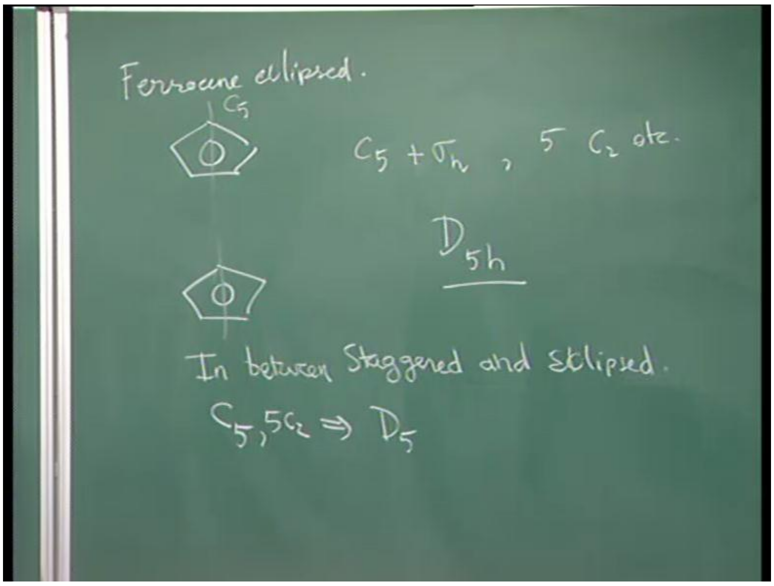

So, if you take anything else in between, so in between staggered and eclipsed, so these two are not exactly in the staggered or the eclipse confirmation, then the group will be, you will definitely have the C 5 axis. So, we will still have the C 5 axis, but you would not have other groups, so it could be D 5. So, you have C 5 and you have 5 C 2 that implies D 5.

So, this example shows you, how the same molecule ferrocene and in different confirmation actually has different symmetry elements, and it belongs to different point groups. This part will become very important, when we are actually looking at the spectroscopic signatures of the transitions of ferrocene.