Symmetry and Group Theory
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Lecture No.4
Symmetry point group: Examples Part III

Hope you received my email I have sent the first class transparency already I have changed it little bit from what we did in class and added little bit more.

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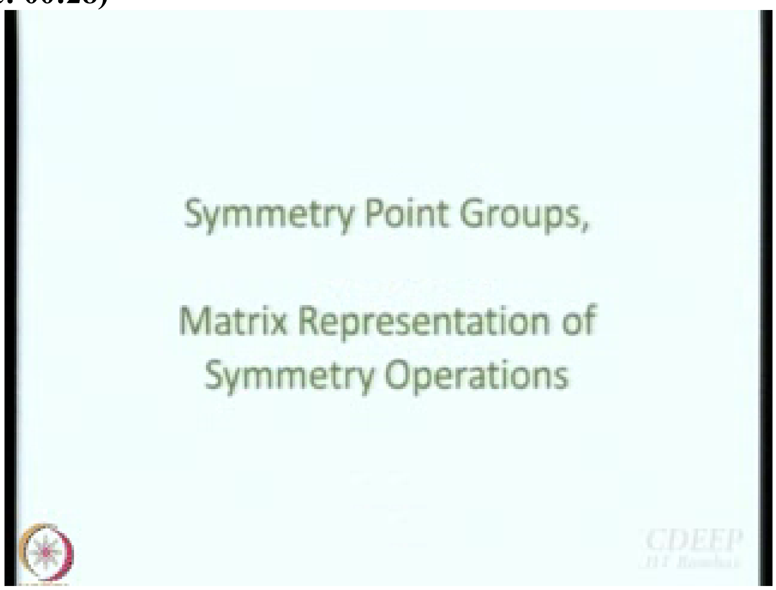

What will be the today we will go back a little bit and discuss where we have stopped and this time with models, yesterday last time ago forgot to bring the models and then we move on a little bit. So, today we talk about some symmetry groups and we will learn how to identify symmetry point groups of molecules no matter how complicated how easy they and then what will be do it we just start talking about how you can use matrices to represent symmetry operation and the next Friday when we come back we will see how we can take that little further.

And that is the only part that we will discuss next day and may be the day after that is the only part where there will be little complicated mathematics please do not get scared it is not very difficult. So, it is really like activation barrier after that is going to be really smooth. What we are trying to do in this course is that we try to understand how things happen. But eventually we try to work out something that will even for even for dummies. Something that would be completely mechanical you can refer to a table and say whatever you have to say. For that we need to do little bit of mathematics please do not get scared.

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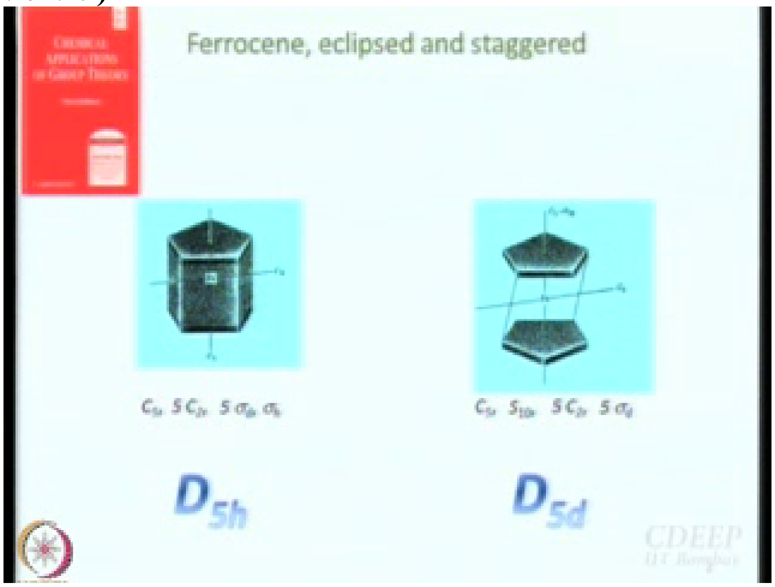

To start with I think we closed the discussion last day with ferrocene and kerosene and ferrocene. So, let us start with eclipse configuration, eclipse is very easy. So, let us say these are the two rings write five member rings one on the top and one on the bottom that is the structure of the ferrocene that is eclipse right. And we will keep it here and we will see it will project in it or not, this is the eclipse structure you do not even see the red thing because the black one is on the top. I think you can identify the symmetry operations already whatever the symmetry operations let us remind ourselves what is the highest order axis C5.

Where is C5? Here right this is C5 ok what else you will have, C2. What is C2 between the rings and oriented like this right between the Rings and oriented like this from on the apex to the mid midpoint and the opposite bond, very easy. If I ask you how many C5 operations are there? How many C5 operations are there? There is 1 C5 element how many C5 operations are there? 4 or 5, 4 because C5 to the power of 5 is just identity right.

What else do we have any other axis ok, whatever plane, two kinds of planes first is you can say Sigma d, what is Sigma d? This is Sigma d right the vertical planes actually they are going to bisect angles between perpendicular C2 axis so called the dihedral planes and you are going to have a Sigma h also. Where is Sigma h? Presences who have lanthanum or ferrous iron whatever it is and parallel to the rings that is Sigma h right.

So, what is the point is then, why d not c because C2 axes are there we have to what account for them. If C2 axis is not there then I could have called them C2h. But here since C2 axis is there we have to account them for them so called d5h ok. Now let us let us talk about the other example with his little more complicated. What is the other example that is the least staggered configuration of the ruthenocene? We have already talked about this C5, C2 Sigma d, Sigma h and there is D5h now let us talk about the staggered configuration ok.

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This figure is the staggered configuration right now what is there they still have the C5, yes I do right, C5 is still there. Moreover this C5 as now become another axis, can you identify that axis. In addition to C5 exactly it is S10 you see the S10 right, take this one right rotate it by 360 degree by 10 it is going to come here that will give you at the top. Now if you reflect with respect to the nonexistent horizontal plane then you get, and then is this red point. And you can work that out for each and every carbon atom that is there ok so far so good, Aachal ok.

So, C5 now becomes h10 also C5 S10 alright What else will be there, will they be seated. Now I think last year you have problem identifying the C2, why because the time was not on that great. Now we have actually have the pentagon's you can see C2 nicely are not. I will just turn the whole thing little bit, now you see, this here it is C2 provided it goes to the central line ok. If I am going to keep it inside the two rings here the whole thing will become very unstable so I would not try it night no need of further amusement.

Please understand that actually goes through the centre of the line now you will see that it is C2 you can see the ring on the top, ring on the bottom this is at the top this is at the bottom right C2 operation with this is going to take this atom, that, that atom here ok then where will this atom go yeah this item will go there as well ok. Now convince yourself that you have a atom to atom mapping for every atom by C2 operation. Look at the structure and convince yourself that works, does it work, it works right.

Convince yourselves take your time, so, that is C2 how many how many C2 will be there v for each C2 so many operations will be there 1 or 2; 1 why because C2 square 1 is again easy do not forget that, so that is C2, is the horizontal plane there, horizontal plane is gone what we have done is we have rotated 1 plane with respect to the other, horizontal plane is completely gone. What about the dihedral planes.

You see the dihedral plane here still, yes still there right, how many dihedral planes? 5 or 10, 5 sure ok, 5 dihedral planes right anything else nothing else look carefully, look carefully something else is there i, right generally i is the poor cousin some of it neglected all the time right axis and planes are glamorous more and we like them more we will talk about them all the time. But i is there, as the result of that the twist that we have given the two planes with respect to each other now this new element i has come which was not there for the eclipse situation ok, so i is there.

I have forgotten to write the i there it seems ok, so I have given the answer point group is D5d. Start D5h anymore right this thing appear that you disturb some amount of symmetry Sigma h is gone. Now it will goes from D5h to D5d point group ok. So, ferrocene clear, sure can you make out the colours black and red, ok black is you want to extend, so I do not need this pencil I will just draw this on the paper maybe so this paper represent the cross section of the S10 axis right. Now what happens if you give what is the meaning of S10 what is the meaning of C10 by how many degrees you are rotating 36, 360 divided by 10. If you rotate it by 36 what will happen this black atom will come to the position of the red atom right but the problem is the black atom is above and the Red atom is below. So, if you just turn by 360 degrees by 10 that is not the symmetry operation right. However if you now this is the axis right, this is the axis. Now if you consider this plane which was the horizontal plane of symmetry for the eclipsed situation.

Now what will happen if you deflect with respect to this plane then whatever is on the top will come to the bottom right. So, see what you see is that you turned it by 36 degrees but now it is not indistinguishable but subsequent to the turning if you provide a deflection with respect to horizontal plane then you will get back to the indistinguishable configuration right that is the S10 for you C5, S10 ok.

CN H2N this is the new symmetry operation comes in new symmetry element that comes in are the result of staggering but the Sigma h is lost Sigma h is something that is higher priority you are actually go from higher symmetry to lower symmetry fine. Let us move on let us talk about tetrahedron. The tetrahedron is the shape that is very close to the heart of all chemists if you understand tetrahedron then you understood a lot of chemistry and this then is tetrahedron for you ok.

So, what we did in the previous class is that to put the tetrahedron inside box and we got the figure like this;

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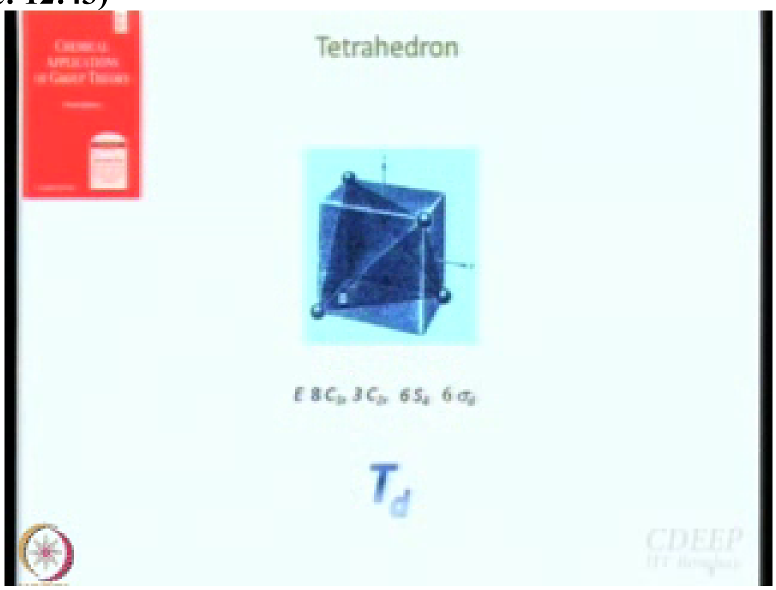

I do not know how clear is the figure, this figure actually from cotton book itself unfortunately net connection is down in my office today so I could not get the prettier picture I think you can figure out right. So, this is your tetrahedron ok now let us see what you have; what is the principal axis of symmetry C3 this is C3 axis. How many such C3 axis are there 4, 1 2 3 4 how many C3 operation would be there 4 into 2, 8 right because we can turn once and then we can turn once again, if you turn thrice then you will have identity ok.

C3 and C3 square 2 operation are there, so XC3 this is the property call platonic solids objects that have more than one principle axis of symmetry, which one is the principle axis of symmetry there are 4 C3 right 4 identical C3 after this we will see a case where we have 3 C2 but you can actually identify a principal axis of symmetry a is the single principal axis of symmetry. Here you cannot, here all the 3 C3 axis or axis can act as; should be considered as principal axis of symmetry because you cannot distinguish between them ok.

More than one principal of axis of symmetry they are called platonic solid that is why it is called HC3 what else was there I think we discussed is in the previous class which other axis is there C6, C6 it is not there, C6 is definitely not there, C2 is there, where is C2 this is C2 this we can show very nicely in the model. You see C2 so it is C3 operations and you have the C2 and how many C2 that is very clear from this figure is it not, there are 3. So, xyz then that is become very convenient xyz axis 3C2 axis 3C2.
Anything else yeah each C2 axis is S4 axis right. So, how many S4 operations will be there, S4 and S4 cube, Maheth, What is S4? You turn by 90 degree right you turn by 90 degrees and then you have to reflect with respect to this plane ok. What will be this if you turn by 190 degree that is S4 to the power 1, S41 if you turn it twice that becomes C2 operation already ok after that you cannot reflect but then you get you can turn it thrice and then you can reflect there are two kinds of C; S4 operations right; Marcovis ok.

6 S4 operations 3 axis 2 operations per axis alright Sigma D where we discussed Sigma D by the by Sigma D is you can see very nicely. One thing to understand here is that you take this to Sigma D you can see that that there are they are perpendicular to each other you actually wants this out when you put it inside rectangle you can work this out nicely. You can see these are perpendicular it is very important to understand these two planes are going to be perpendicular right.

How many such planes will be there 6 or 8, 6 actually the answer is in front of you sorry the one thing that we sometime forget that we should not forget is that whenever we teach symmetry operations we should not forget the obvious and that is E anything and everything is E, E means identity or C11 whatever way you want to call it. You take a tortoise and turn it around it 360 degrees is a symmetry operation for the tortoise. May be rhino would have been a better example.

Because I as we see later when you use deep theory very important that we work with the order of the probe or else will be the total number of symmetry operations this is also a symmetry operations if you leave this out then only one less than order so you should not forget E. In mathematics if you forget one or for multiplication or zero for addition things are not going to be that great is it not ok fine.

That is the tetrahedron in fact I ask you to work this at home is it not how many operations are there in the tetrahedron. I hope some of you did it even if you did not then answer is now in front of you alright. So, this is called TD and depending on which operations are there which operation is not there you can a variant of Td, Th and so on and so forth that you can look after in your Cartons book.

Now let us talk about my favourite molecule Allene, we just talked about Allene in previous class right these is a Allene looks like. I will take this atoms of this is Allene ok. So, see once again this plane and this plane they are perpendicular to each other is it not. You see that it is basically like you started with tetrahedron ok and somehow we will be able to pull it in such a way that you have been able to bring in a distortion like this.

So, I think you will understand now that Allene will have symmetry operations symmetry elements that will somehow related to these of tetrahedron. It is just that many of the symmetry operations would have been destroyed as a result of distortion ok. What are the symmetry operations that are that are there in Allene. I can write down the first one ok and you tell me what the second one is C2, where are the C2.

This is a C2, this is very easy, this is inside the axis this is a unique C2, you say this is a C2. Now there are 2 other C2's, where are the other C2's, so see it very nicely you if you hold it like this, hold it like this ok now think of what is easier for me horizontal or vertical maybe horizontal ok. Think of these axis defined by these two index fingers of mine, can everybody see. Now if I see what you have the one towards you on the top, look at the two atoms are the towards on the top and two atoms towards you.

The top one is towards you are right and bottom one is towards your left right justifying on that the top one is towards your right and the bottom ones towards your left ok. I turn it by 180 degrees see what has happened, because the atom towards you one on the top is towards right and the one on the bottom is towards your left ok. You watch with your both eyes one eyes is not going to help.

You see this yes or no is that yes or no ok sure C2 Sumanth right sure ok the other C2 is perpendicular to it once again do not forget look at the other towards you one of the top towards your right, right turn it you will get back the same thing ok so 3 C2's 1 then you just that you have to hold it like this 2 and 3 and do you noticed that these C2 axis are still perpendicular to each other is it not, they are still perpendicular to each other is just that is a long axis and there are two short axis ok.

Any questions, no questions fine so ok this is also S4 right, long axis is also S4 right, turn it by 90 degrees and then reflect you get back the same thing ok. S4 and 3 C2 fine what are the planes do you have any inversion symmetry no inversion, start from here it go to the centre and go there nothing. What else what about planes do you have plans? How many S4 will be there, what happens if I; this is S4 right, so this is 1 and this is 2 this is not a symmetry operation you go there it does not make a difference there is only one S4 ok.

Now planes is any other planes, so many place in tetrahedron only 2 have survived ok. What will be the point group, principal axis symmetry is there, what is the principal axis of symmetry C2 do we have perpendicular C2, yes so that as to be D2 and is there a horizontal plane, no, dihedral plane yes so it is D2d alright, Allene is simple. If you understand Allene if you go on your new projection the way I have shown to you is basically a new end projection. You draw a circle on one line this way and one line that way and that is new one projections ok.

Now let us make this little more interesting or little less interesting new one where it becomes let it be some more substitutions in organic chemistry to do it is not that easy for me that it is very easy I just to put in two white sphere. Now let us see this is the case this is hydrogen this is chlorine or such thing ok substituted in Allene.

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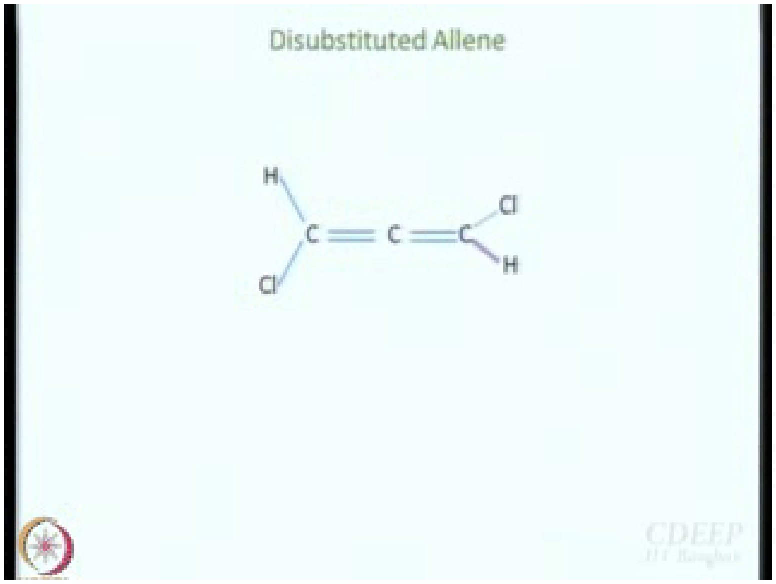

E is there, is there anything, C2 this is C2, no then ok. What about this one, hydrogen is towards your top right turn it when it is at your top, however look at this one, towards you chlorine is at the bottom and towards your right, turn it you get the same thing. So, one C2 will survive nothing else survive, so whose turn it will be C2 or C3? C2. What about this if two substitutions are on the same carbon then what will happen, which C2 is there, now long axis is there right, that is C2, other C2 are obviously not there.

Is there anything else, Sigma, where is Sigma? Is this Sigma is there any other Sigma, this is also a Sigma. So, this is C2 this is one plane this is another perpendicular plane inverse of symmetry is not there E is of course there that is the point group, C2v have you talked about any C2v molecule earlier, water right. Now look at this carefully forget the rest of the molecule something is look like water here I forgot this part of the molecules that something looks like water here perpendicular to each other.

So even though chemically there is nothing similar between what di-substituted Allene that belongs to the same family as far as symmetry is concerned. And if you think of CH2 CL2; CH2 CL2 does it not have the same symmetry, once again you have one C2 one plane here, one plane here CH2 CL2 is also C2. So, water, CH2 CL2 and di-substituted Allene is on that same carbon they all belong to the same point group that is C2 and you also see those two planes not equivalent they belong to the same class right fine.