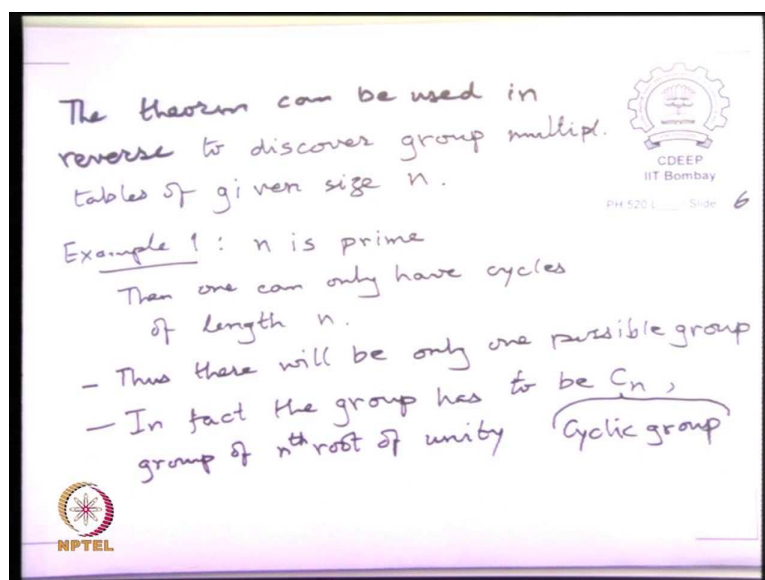


Theory of Group for Physics Applications
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Lecture – 10
Cycle Structures & Molecular Notation – II

So, the theorem can be used in reverse. So, I hope you are convinced as far as at least group G is concerned; not the generic regular representation, but so, long as these are elements that represent a group. So, for that set, it is true that they have to be broken up into cycles of equal length ok. So, the theorem can be used in reverse.

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to represent it to discover group multiplication tables of a given size.

So, simplest example, if n is the prime number, then you cannot subdivide into groups of equal length as you cannot subdivide into any, it does not have any divisor. So, if n is prime, then one can only have cycles of size n length, I think that called length. So, there is only one way of writing out and you will have only one possible group because well, I am asserting this without proving, but it is easy to see why because you will have to keep changing to represent. So, if you can have cycle only your size n and you have to have n elements and you have to change, then the only way, you can do is get only one group out of it, you cannot get two groups out of we are doing this.

Furthermore; therefore, it is also easy to see that this will be nothing, but the Abelian group C_n ; it will be just the n -th root of unity. So, that is quite interesting and satisfying that after all, this fancy thing; we have some specific. The group has to be just the cyclic group of that is the that was the word I was trying to remember cyclic group of size n , next you can see example 2, although, it is a bit simple again.

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Example 2: We can check that C_4 and Klein group are the only groups of order 4.

| C_4 | Klein gr. | |
|----------------|---------------|--|
| $(1\ 2\ 3\ 4)$ | $(\)(\)$ | This exhausts kind of cycle structures ... intuitively |
| $(\)(\)$ | $(\)(\)$ | |
| $(\)(\)$ | $(\)(\)$ | |
| $e = (\dots)$ | $e = (\dots)$ | |

We can check 3 4 cycles and 1 pair of 2 (es does not work. Hence there are only such groups.

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We can check that C_4 and Klein group are the only groups of order 4 because we already checked that C_4 has this thing; $(1\ 2\ 3\ 4)$ and then some split 2 cycles and then again another cycle form and of course, identity identity.

So, e equal to something, but they split into 2 elements of size 4 and 1 element which is 2 cycles; the Klein group is as we claimed breaking up into $(3\ 2)$ cycles and the identity, there is no other way of dividing 4 ok, there is no other way of partitioning 4. So, this exhausts all the groups that you can possibly get at level 4 of size 4 maybe, I should fill in, but just to save time you can fill in these ok.

So, this exhausts kind of cycles, you can make; there is a little more that needs to be sent to make this watertight which is. So, why I do not I have 2 elements with 2 cycles and then 2 elements with 4 cycles, see here, we had 3 elements which were essentially 4 cycle and only 1 element 2 cycle here, we got all 3 of them, 2 cycle. Is it possible to have 3 elements of in a 4 cycle and 1 in a 2 cycle, the answer is no ok that you have to check.

But that has to do with equivalent classes the fact that equivalence classes retain the size. So, I will just say it is incomplete proof right now, but intuitively this is clear, we will see the detail another time when we are doing something else you can. So, thus there are only. So, we can check three 4 cycles and 1 pair of 2 cycles does not work. So, hence there are only 2 such groups. So, now, there are 2. So, I said we want to do 3 things out of which one have completed, but it has taken a little longer than I thought. The 3 things can consisted of doing this.

Then this theorem; these observations that we are making can actually we generalized and made much more interesting and so, there is a theorem that one can prove. So, I am launching it into it, we will see how we cover all the 3 parts. So, and generalization comes from introducing particular ways of writing out cycles.

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This kind of process can be generalised to larger size groups.

Introduce notation for cycle structures

Given π which has ν_k cycles of size k

--- ($\underbrace{\quad}_k$) ($\underbrace{\quad}_k$) ... ($\underbrace{\quad}_k$) ---

$k_{\max} = n = |G|$

Introduce $\lambda_k = \sum_{k=1}^n \nu_k$

Thus $\nu_k = \lambda_k - \lambda_{k+1}$

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This can be generalized to this kind of process to larger size groups without having to write out all the possible cycle structures explicitly, by a theorem that says that the number of the number of partition number of ways of partitioning is what gives the possible number of groups you can have. So, by introducing a concept of partitions well partitions for a number is clear.

So, we introduce this notation for cycles. So, given up , which has ν_k cycles of size k so, what we mean is suppose I have a cycle of size k , and I will keep counting how many

these are and this list is λ_k and then there are other things. I will do half of it now and then half of it next time, I will tell you the main result, what we do is we introduce

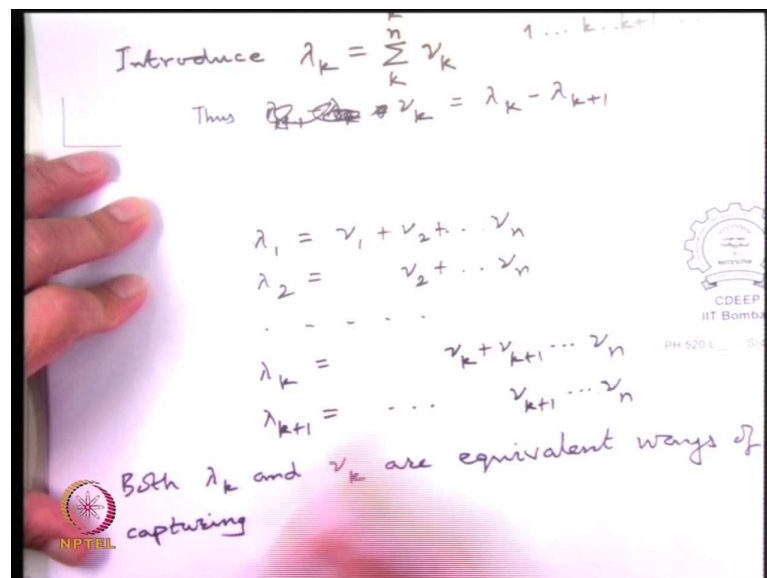
$$\lambda_k = \sum_{j=k}^n v_j$$

So, note that the largest k is of course n , the size of longest cycle is the order of the group.

So, the sum in λ_k can go only up to n , but the trick we are doing is starting with some k and going up to n you will see the advantage of doing this. So, thus we find $\lambda_k - \lambda_{k+1}$, which will be equal to v_k because $(k+1)$ is a summation that will start with $k+1$, right. So, one way of remembering this is let us write like this as $k+1$. So, the λ_k starts with k , λ_{k+1} starts with $k+1$. So, $v_k = \lambda_k - \lambda_{k+1}$. So, if I write λ_k or I write v_k the description is equivalent ok.

Whether, I write the how many how many cycles of size k occur and remember, the λ_k is or construct out of them the differences or what we have actually done is we can think of it also like this that, there is the $\lambda_1 = v_1 + v_2 + \dots + v_n$.

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λ_2 will start with v_2 and go up to v_n like this. So, this is what it is and therefore, the $\lambda_1 - \lambda_2$ will be simply equal to v_1 , we will start with v_{k+1} and go up to v_n . So, $\lambda_k - \lambda_{k+1} = v_k$. So, there is a both λ_k and v_k are equivalent ways of writing out the cycle

structure of how should we say capturing the cycle structure because the conversion is unique right this.

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Introduce $\lambda_k = \sum_{k=1}^n v_k$

Thus $v_k = \lambda_k - \lambda_{k+1}$ (boxed)

Both λ_k and v_k are equivalent ways of capturing the cycle structure

Now note $\lambda_1 + \lambda_2 + \dots + \lambda_n = n$

check $\lambda_1 + \lambda_2 + \dots = \sum k v_k = \text{no. of total elements in all cycles} = n$

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So, linear relation between λ_k and v_k , so, now the advantage of writing in terms of λ_k is now the following if I sum all the λ_k , I get back n why is that true? Well look at this explicit way that we wrote out this, if I start summing the λ_k , I will get λ_1 exactly once, I will get λ_2 exactly twice.

So, in other words λ_k is actually equal to $k v_k$. So, as we saw λ_1 will occur twice in this sum λ_2 will occur thrice. So, actually it amounts to $\sum k v_k$ the cycle of size k will occur exactly k times in this sum of the λ_k . But that has to reproduce the total thing n . If I count the number of ways that cycle k th cycle occurs the sum of all the lengths some of this is actually sum of all the cycles $\sum k v_k$ equal to number of total elements in all cycles.

So, it exhausts all the elements which is equal to n . So, this means that. So, now, one has to one can establish a relationship between the kind of cycle structures one can have and the order of the group.

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Thus we can say: The kind of cycle structures possible for a group of order n = The number of ways of partitioning n

$$n = \lambda_1 + \lambda_2 + \dots + \lambda_n$$

Note many λ_k can be zero
Also many λ_k can be zero.

So, thus we have is equal to the number of ways of partitioning n . Because you write out what is meant by partitions $n = \lambda_1 + \lambda_2 + \dots + \lambda_n$ try to partition it in all possible ways. So, some of the λ_k can be 0 note many λ_k can be 0 and many λ_k can be 0. When successive λ_k have same number of cycles and λ_k is same for k and $k+1$, then the difference is 0. So, I want to leave this theorem here right now, because I think some of the things we need to go over again before we capture all the essence of this theorem.

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$$\begin{aligned} \lambda_1 &= v_1 + v_2 + \dots + v_n \\ \lambda_2 &= v_2 + \dots + v_n \\ &\vdots \\ \lambda_k &= v_k + v_{k+1} + \dots + v_n \\ \lambda_{k+1} &= v_{k+1} + \dots + v_n \end{aligned}$$

Both λ_k and v_k are equivalent ways of capturing the cycle structure

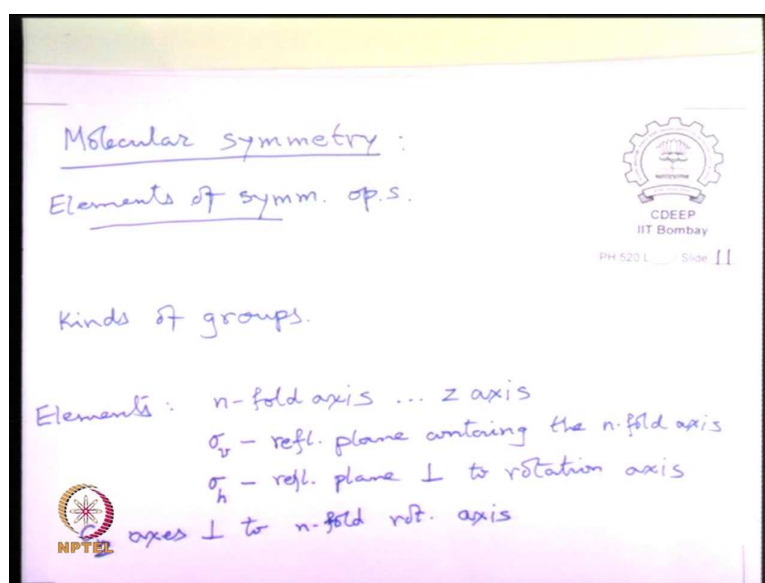
Now note $\lambda_1 + \lambda_2 + \dots + \lambda_n = n$

check $\lambda_1 + \lambda_2 + \dots = \sum k v_k = \text{no. of total elements in all cycles} = n$

So, for the time being, I will just leave you with this enumeration and summation exercise and we will see later; what is the, for the significance of this in trying to determine structures of groups as a general thing.

So, with this, we finish these 2 parts of today's lecture, what I am going to do next is symmetry notations in chemistry : molecular symmetry.

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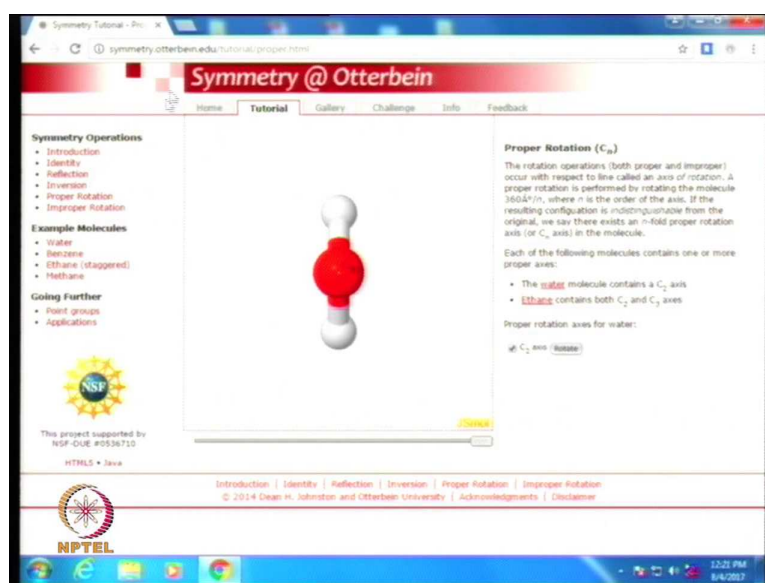
So, it turns out that one can capture all the possibilities in a small list. So, let me begin by saying the elements of symmetry operations and then there is kinds of groups the elements of symmetry operation are things like rotation, reflection and so on and what combination of rotations and few reflections mix up a set a group is there are notations for that. So, elements of symmetry groups are as we saw first, n fold axis, which we usually represent by z axis and so, let me see if I can switch between this and this. So, let me first right, this list here and then we will see the simple example.

So, n fold axis of rotation, then there is something called σ_v , this is a reflection plane which contains this vertical axis itself ok. So, think of water molecule and I can draw a vertical axis which is the 2 hydrogens that reflection. So, there is a reflection plane containing the symmetry axis, but there can be another kind of reflection plane which is called σ_h and these are this is a reflection plane perpendicular to the reflection to the rotation axis. Then other kind of transformations are having a C_2 axis, sorry, a C_2 axes perpendicular to the n fold axis. So, you think of molecule which has I think I should

show pictures. So, I have a axis of rotation, but I have perpendicular axis which flips things in such a way. So, a C_2 axis only just rotations which are perpendicular to it which also keep it invariant.

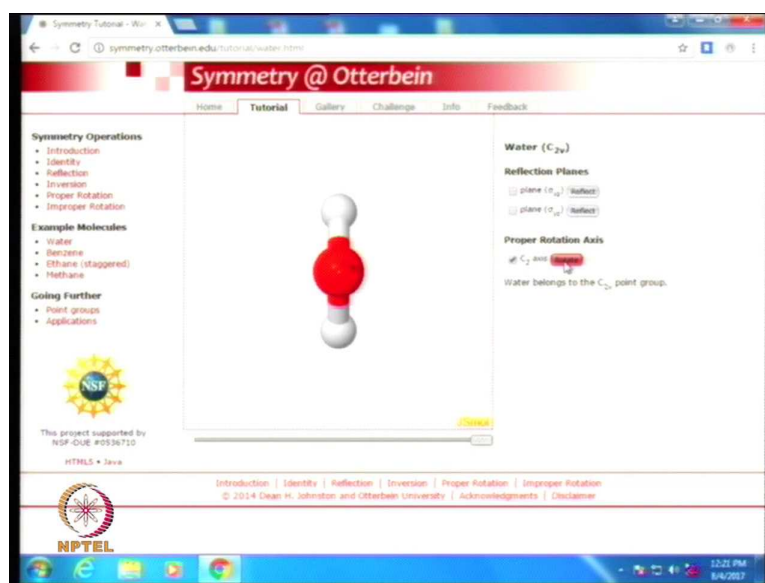
So, take a square. So, you can have a fourfold axis of rotation, but you can have axis passing through the diagonals and axis bisecting the square, around which you can do 180 degree rotations. So, those are C_2 axes perpendicular to the n fold rotation axis and then there is a nomenclature for the groups.

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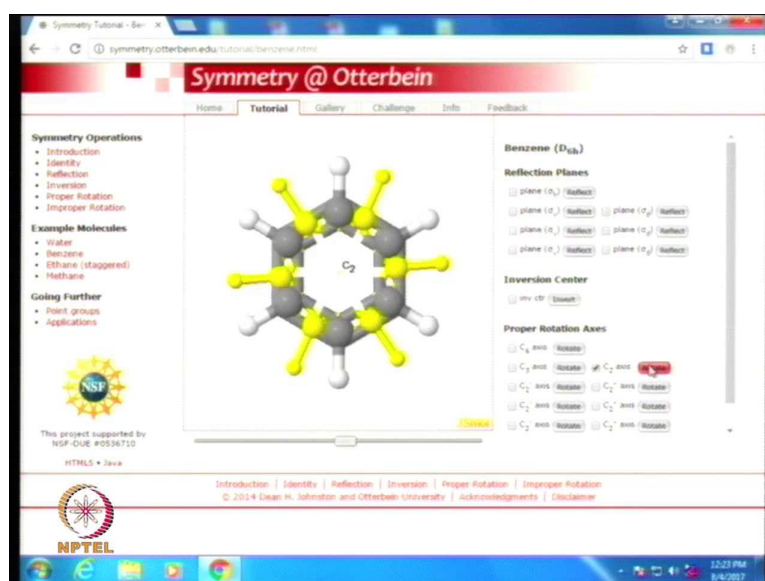
So, let us look at some examples. So, take note of this place university called Otterbein it is in Ohio, I think and they are maintaining a complete kind of tutorial of symmetry as far as used in chemistry. So, this is the water molecule and it has a C_2 axis.

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So, it passes through and. So, z axis is pointing towards us it has a, it has 2 planes which are both actually σ_v in the notation, I just said one plane passes like this. So, one is x z in which you can reflect or there is a y z which does not do much, right because it is just passing like this and it is a planar molecule. So, mole; so, every planar molecule always has a a plane which trivially reflection into itself let us look at benzene ok. So, this has all kinds of elements.

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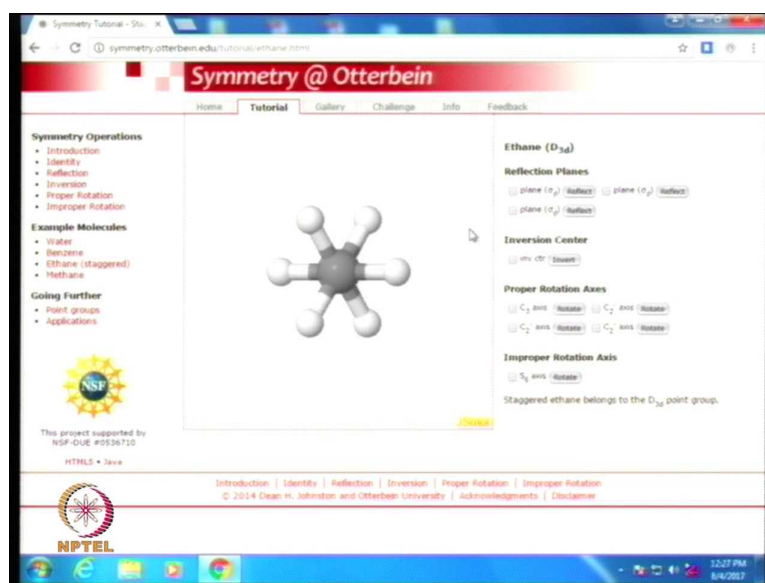
And I did not so far say about inversion. So, we will say see everything here. So, first of all it has, of course, as you know famously the 6 fold axes. So, it rotates ones well it shows it shows only the first element, then of course, there is a C_3 axes which is just going to do this it is a combination element.

C_2 axes which is rotation I do not know what C_2' is. So, this is my C_2 axes as I said. The C_2 axes which is supposed to actually be perpendicular. So, the this C_6 axes, C_6 axes is pointing into the plane of the picture whereas, this C_2' is perpendicular to it and there are of course, 3 C_2' s as you may imagine one in each of these, the third one is there and then there are C_2'' . So, there are 3 C_2 axes which pass through the mole through the atoms and another 3 which is dihedral cut the bonds that. So, this C_6 , C_3 and C_2 are only elements of the cyclic group C_6 , but this primed axis are the ones that are cutting the bonds into half. Other than that there are all these σ_v planes, there is $\sigma_{v_1}, \sigma_{v_2}, \sigma_{v_3} \dots \sigma_v$ means a plane that contains the n fold axis of rotation.

So, one of them; so, our axis of rotation is z and is coming out of the plane of the screen, σ_y does this reflection, another which will do this. So, this σ_d planes are all passing through these and there is another category of which are called σ_d . So, the σ_d are called dihedral planes. Dihedral because they take the; so, instinctively these are the simpler planes, right. So, let me remove this. The once that pass through the atoms are the important planes to consider additionally there is a plane which divides 2 of those. So, these 2 orange planes are divided by this yellow plane. So, the plane that falls in between 2 of those category of planes is called a dihedral plane ok. So, it is called σ_d and does it do something well. So, that reflected around that plane.

So, this is the whole list and finally, there is the very simple σ_h plane which is passing through this planar molecule and if I reflect let us see what they show not much ok. So, because it is just anyway you cannot distinguish upper part of carbon molecule for lower part, but there is that σ_h . So, this introduces the all the notations, there are σ_v , the σ_h and σ_d 's whenever, there is a C_2 's, it means that they are flip x 180 degree rotation axis perpendicular to the main symmetry axis of rotation.

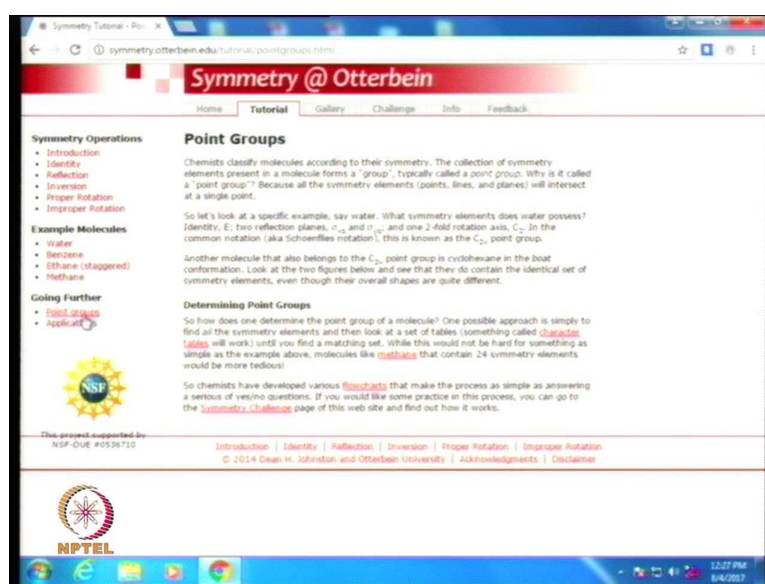
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So, ethane oh and the groups are written here. So, sigma water is essentially called. So, that was the other part, I was going to introduce which is the list of the groups that you get eventually. So, thus C_n and C_2 's etcetera are elements of the symmetries, C_n symmetry, but finally, we have nomenclatures for groups.

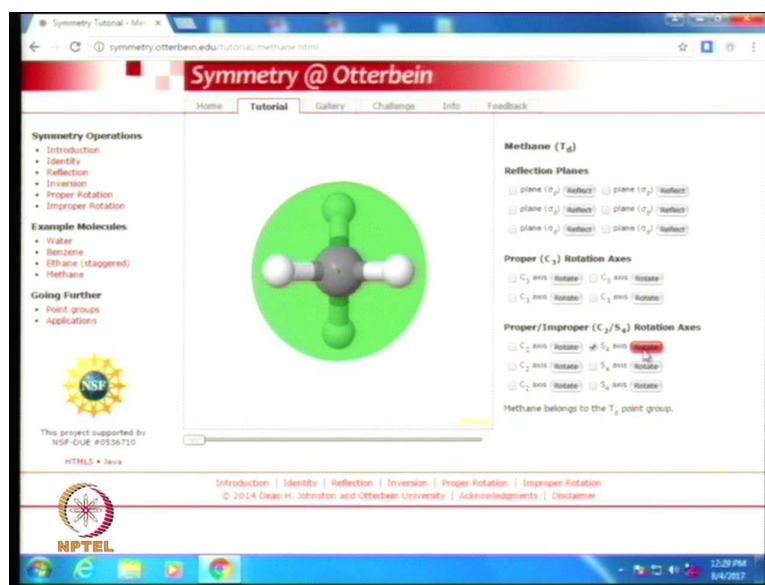
So, this is called C_{2v} as Firstly, it is C_2 , because it has this C_2 axes of rotation and it has vertical planes of symmetry, I was looking for whether the ammonia molecule.

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So, well methane. So, there is there also elements like methane which are extremely symmetric because they have extremely large extend of symmetry there just this 4 carbons.

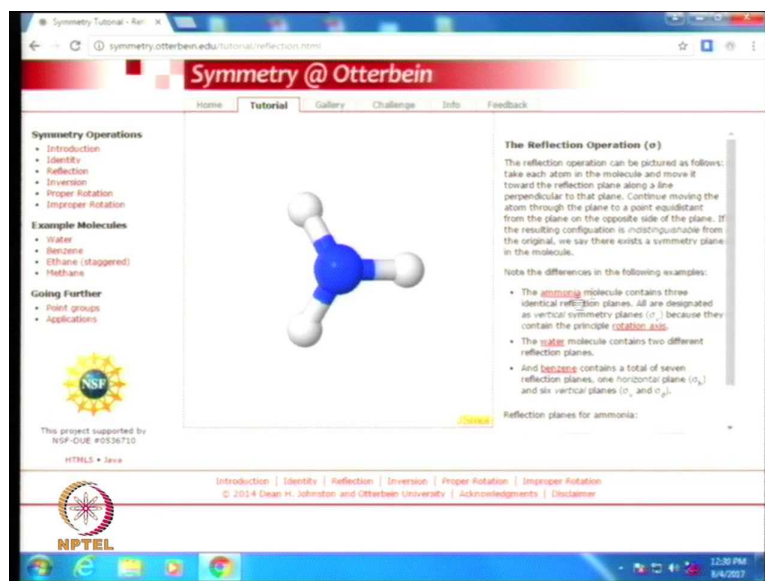
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Here you have to imagine these 2 carbons has coming out of the plane and these 2 bonds going into the plane and it has 24 symmetry elements, but essentially generated by fewer one. So, essentially there; there is a reflection plane of this type, which contains 2 of the carbons at a time sorry hydrogens at a time, and it has C₃ axes which is an interesting axes, it passes through this and through one of the hydrogens. So, if you rotate, it rotates like this, but then of course, you can do this with any of this hydrogens right. So, there are 4 such C₃ axes and then there are interesting C₂ axes, which are not intuitively clear at first ok. So, this goes through this and if I rotate this all the way around, you get here and right you can see it here and then there is an S₄ axes.

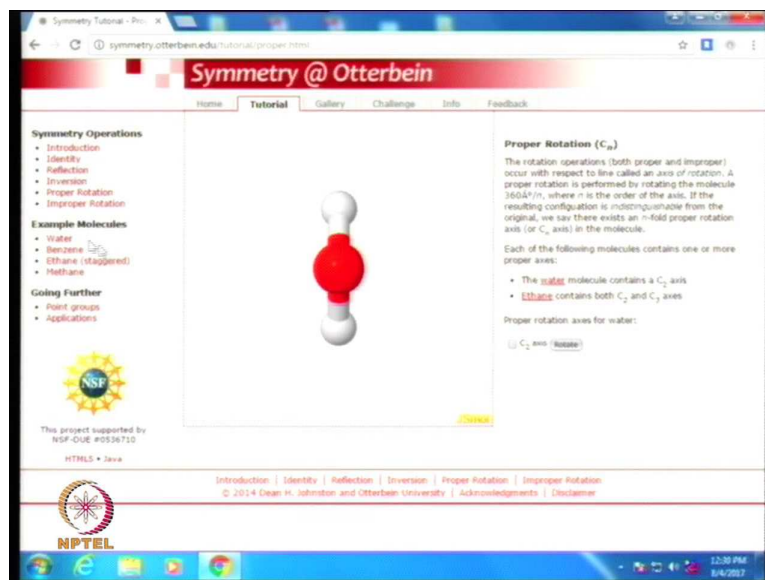
So, that is another symbol S. So, when they used S it means a rotation followed by a reflection in the perpendicular plane. So, it is an improper rotation we will do again next time, we will start with all this. So, the S₄ axes are basically a 90 degree rotation followed. So, they are trying to probably show it. The rotation axis is going to be this and then there is going to be a reflection in this. So, note it; first it is going to reflect in this plane afterward the thick plane, it is going to first rotate by 180 degrees there and then it flips it ok, then it comes back.

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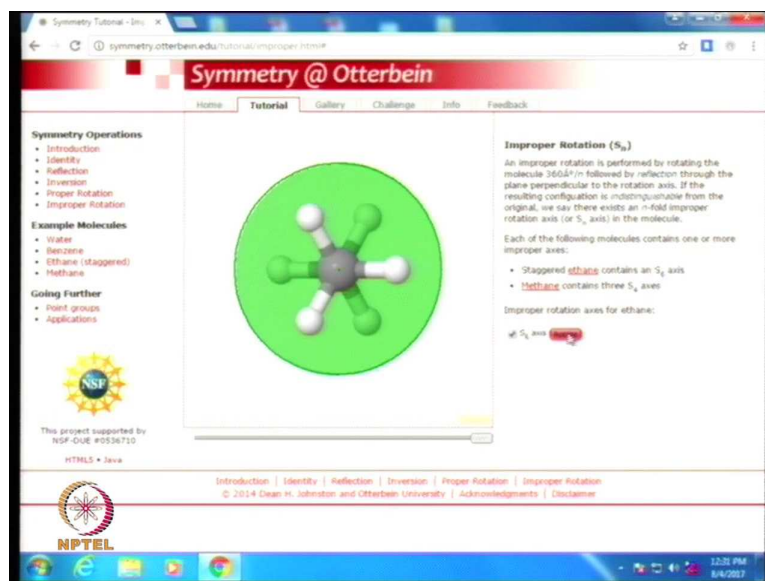
So, this as much larger group and they have here shown individually also what is meant by reflection, , but there is no, here ammonia; ammonia is the good molecule.

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So, proper rotations and improper rotations, it will show all of this.

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Improper though methane, we already say well we ethane we some methane, but the case of ethane will also have S_6 axes, right. So, what is happening? You see what is happening they are rotating this up to here, which is $2/6$ rotation and then reflecting into the green plane, then you get back the molecule. So, last part is the reflection. So, this is called an S kind of axes, a rotation and reflection ok. So, we will see more about this next time.