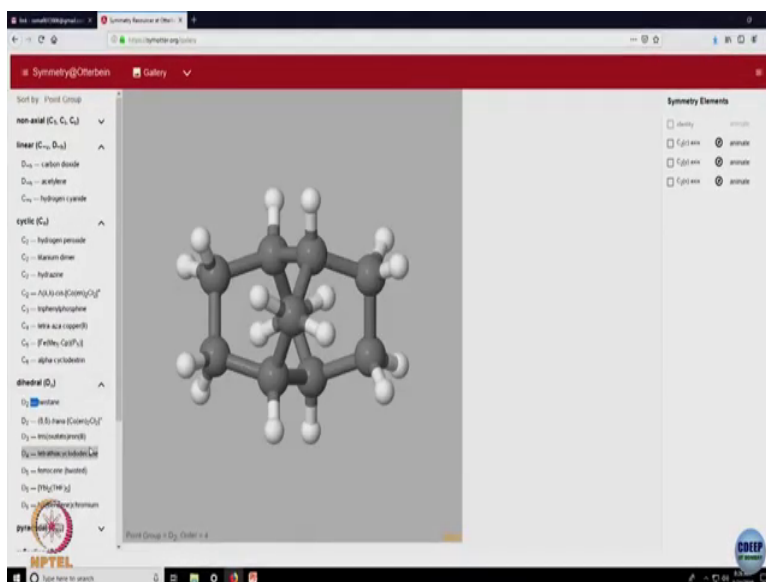


**Group Theory Methods in Physics**  
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**Lecture – 14**  
**Examples of Molecular Symmetries, Proof of Cayley Theorem**

So, someone was asking what molecules have, what symmetries and so once I thought if you get a feel of it, so this (Refer Time: 00:24) website is very beautiful.

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So, you can start going on to see what are the molecules and then there is animation on the right hand side, you can do the animation to see whether it has any other you know this is the  $C_2$  symmetry where if you keep track of one you can see that it goes to the diagonally opposite point and so on. So, you can see the mirror reflection for example along the sorry,

this is C 2 along the y axis ok. So, C 2 along the y axis this left right symmetry you know, it goes can you see it, it is the left right symmetry.

So, this is one way in which you can see that there are various compounds or you can call it molecules in chemistry, where they first figure out what is the symmetry possessed by the molecule. This molecule it need not be C 2 right it could be much more than that, but they try it out and make sure that what is a maximal symmetric group it has. So, I thought let me share this I did send this link, how many of you tried it? I do not know how many if you tried, but there was a super symmetric tutorial which will give you a hands on you know what are I tried to do it in the class.

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The screenshot shows a web browser window with the URL [www.chemeddl.org/symmetry](http://www.chemeddl.org/symmetry). The page title is "Symmetry Tutorial - Introduction". The main content area contains the following text:

Welcome to the world of symmetry! Symmetry plays an central role in the analysis of the structure, bonding, and spectroscopy of molecules. In this tutorial, we will explore the basic symmetry elements and operations and their use in determining the symmetry (point group) of different molecules.

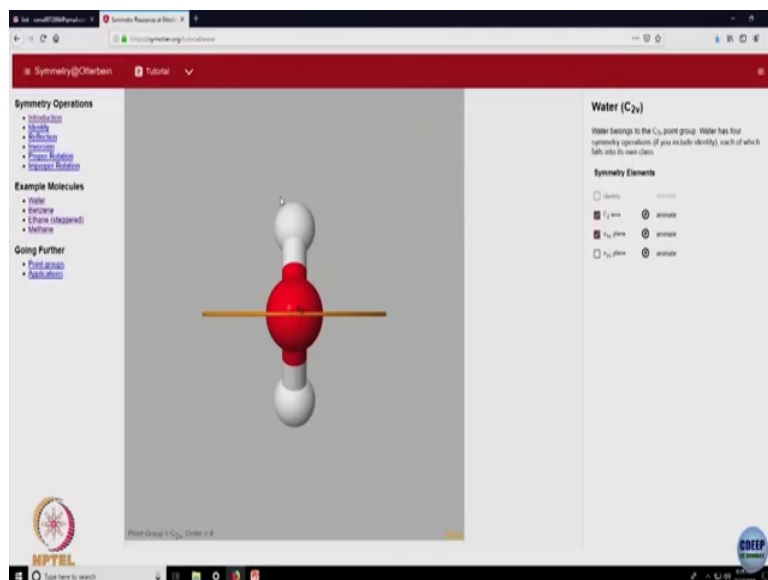
The symmetry properties of objects (and molecules) may be described in terms of the presence of certain symmetry elements and their associated symmetry operations. The various symmetry elements and operations are described in the table below.

Element	operation	symbol
symmetry plane	reflection through plane	$\sigma$
Inversion center	exchange every point $(x, y, z)$ to $(-x, -y, -z)$	$i$
proper axis	rotation about axis by 360/n degrees	$C_n$
improper axis	rotation by 360/n degrees followed by reflection through plane perpendicular to rotation axis	$S_n$

The next few pages introduce each of these symmetry elements with example molecules having each type of symmetry. Select the checkboxes to display the individual symmetry elements and press the buttons to animate the corresponding symmetry operations.

Following this, there are several pages of molecules that show all of the symmetry elements present in a particular molecule. These collections of symmetry elements are set up so you can assign a particular molecule to any point group or refer to a particular symmetry point group.

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But here, you could try and do the C 2 axis, animation, you can see that both the hydrogen sorry hydrogen atoms move from one to the other if you do a sigma x, sigma z plane then you see that those two atoms exchange the positions is that, ok.

So, you can get some feel on doing the animation yourself and see what molecular symmetry is all about ok. So, I am not getting onto it there are point groups and you can check out various things to get your clarification on the notation. I have confined to something called Schoenflies notation, sometimes these people follow some other notation by putting you know two bar which means bar means mirror and so on.

So, let us not get into new notations let us confined to the Schoenflies notation, where c n means principal axis is n-fold axis. And once I put c and v then we will have a vertical mirror containing the axis c n h means, a vertical a mirror horizontal mirror which is perpendicular

to the axis. Let us follow that notation and we are not going to follow anything other than this notation in this course, fine.

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**Symmetric Group**

To Prove: Conjugation preserves the cycle structure

$$\sigma = (a_{11} \dots a_{1s_1})(a_{21} \dots a_{2s_2}) \dots (a_{t1} \dots a_{ts_t})$$

$$\pi = \begin{pmatrix} a_{11} & \dots & a_{1s_1} & a_{21} & \dots & a_{2s_2} & \dots & a_{t1} & \dots & a_{ts_t} \\ b_{11} & \dots & b_{1s_1} & b_{21} & \dots & b_{2s_2} & \dots & b_{t1} & \dots & b_{ts_t} \end{pmatrix}$$

$$\pi^{-1} \sigma \pi \text{ on } b_{11} : b_{11} \xrightarrow{\pi^{-1}} a_{11} \xrightarrow{\sigma} a_{12} \xrightarrow{\pi} b_{12}$$

$$\pi^{-1} \sigma \pi = (b_{11} \dots b_{1s_1})(b_{21} \dots b_{2s_2}) \dots (b_{t1} \dots b_{ts_t})$$



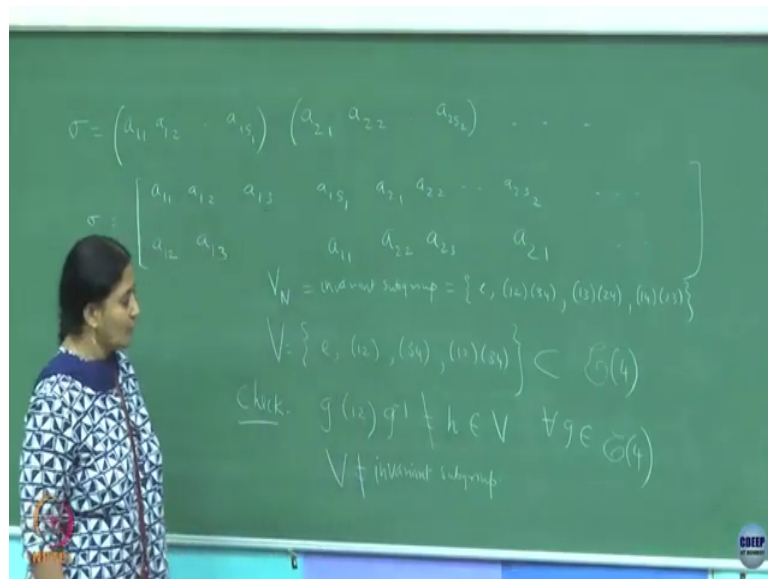
So, so far a warm up on how to look at the molecular symmetry as I said I wanted do a couple of problems I said tutorial today. One of the things which I passingly said is that when you do a conjugation of element. The conjugation of the element suppose the element in the symmetry group of degree n has some cycle structure, if you do a conjugation I said that the cycle structure remains unaltered, it will go to a new element, but the cycle structure remains unaltered, right. So, we can write the element in the cycle structure so if you look at the cycle structure ok. So, aim is to prove conjugation preserves the cycle structure, ok.

So, suppose you take an element in the symmetric group looking at this element you will have you know the there is a s 1 cycle s 2 cycle s t cycle I am not even telling what is the number

of that, this is an element which you have. Once you have this element and now let us take that; so, we know the set of elements in that symmetry group, right. So, you have I have calling it as a 1 1 and those are the elements which are the objects on which you do the permutation, and the objects are such that a 1 1 object if you do a sigma, sigma by sigma you mean a 1 1 goes to a 1 2 in this notation you could have written it that way right.

Let me write it for you. Sigma I have written it as a 1 1, a 1 2, a 1 s 1, a 2 1, a 2 2, a 2 s 2 and so on right, the same thing I could have written here.

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In this notation, only thing you have to remember is that this cycle structure means this group element is a 1 1 will go to a 1 2, a 1 2 will go to a 1 3 right and then a 1 s 1 will go to a 1, clear. And similarly a 2 1 will go to a 2 2, a 2 3 and this one will be.

Student:  $a_2$ .

$a_2$  and so on. So, this is the long hand off writing the permutation element in the symmetry group whatever is the degree is dictated by  $s_1$  plus  $s_2$  you know so many elements, that will be the degree of this permutation group. And, for that particular permutation which is written in the cycle structure you can right along hand like this, clear. Similarly, I have another element which I have written it in the long hand. I am not saying what is  $b_1$ ,  $b_{s_1}$  some other elements, it does not need to be the cycle structure  $a_1$  will go to one of those elements from the set and I am just calling them to  $b_1$  and so on.

We want to prove conjugation preserves the cycle structure that is the motivation. So, we want to do  $\pi^{-1} \sigma \pi$ ;  $\pi$  some arbitrary element permutation element in the same symmetric group of degree which was there for  $\sigma$ , ok. If you do  $\pi^{-1} \sigma \pi$  on  $b_1$ , so let us take 1 of the element  $b_1$ , ok.

So if you do  $\pi^{-1} \sigma \pi$  on  $b_1$  what does  $\pi^{-1}$  do on  $b_1$  if you look at it here, it is a reverse operation;  $b_1$  a specific element  $b_1$  under an inverse of  $\pi$  they will go to  $a_1$ . Under  $\sigma$  you know  $a_1$  will go to  $a_2$ , again you do a  $\pi$ , if you do a  $\pi$  on  $a_2$  it goes to  $b_2$ .

So, what have I essentially achieve is that the element  $b_1$  under the conjugation operation goes to  $b_2$ .

Student: (Refer Time: 08:41).

So, I am just taking one object in the object of degree  $n$  and I have defined what is the  $\pi$  operation, I have defined what is a  $\sigma$  operation. So, one object which I am just looking at it I am calling it as  $b_1$ . The  $\pi$  operation  $\pi^{-1}$  operation  $b_1$  I know what it will do that, that is what I am proved.

Student: (Refer Time: 09:06).

No no, it is just a specific exam see I am not even giving us an example any arbitrary permutation element will have some cycle structure. For example, let me take an  $s$  one cycle structure  $s$  two cycle structure and so on.

Student: (Refer Time: 09:21).

Which cycle structure no, I am not done it I am not done it, I am doing it for a particular element I am not finished the whole thing, ok. So, I have just shown that a specific element of so many objects if you take and if you do this conjugation operation that specific element, you can take any element; you could have taken  $b_2^{-1}$  or  $b_1 s^{-1}$ , I do not care, ok. You can take any element if you do the  $\pi^{-1} \sigma \pi$ , you will show that the corresponding that set of series of operation which I do will take you from for this particular example of  $b_1^{-1}$ , it will take you to  $b_1^{-2}$ .

If you are taken  $b_1^{-2}$  it would have gone to  $b_1^{-3}$ . So, what I am trying to show is that if you go to  $b_2^{-1}$ , if you go to  $b_2^{-1}$  it will not give you any of these sets, ok. So, this by induction if you do this by induction you can call it a  $b c d e f g h$  you know, you can call any letters I do not care, but what I am saying is that subset of  $s^{-1}$  letters under conjugation will only mix only those subset of  $s^{-1}$  letters, yeah.

Student: Ma'am  $\pi$  was (Refer Time: 10:53) operator.

It is an operator you can take I have  $n$  objects and I do  $\pi^{-1}$  on that  $n$  object and then I do a  $\sigma$  on the modified  $n$  objects, that modified  $n$  is permutation of those  $n$  objects and again a  $\pi$  on it.

Student: I was saying that (Refer Time: 11:15) operate  $\pi$  and (Refer Time: 11:17)  $\sigma$ .

You can do that also, you can check it out also, do that also ok. So you can do whichever way you want and I am just trying to say that if you started with a sigma with some specific cycle structure a conjugation will not all to the cycle structure, that is all I am trying to motivate you that. This is the steps even though, I have looked at a specific element in this order of pi inverse sigma pi, you can see that the conjugation preserves the cycle structure. So, that is why I said pi inverse sigma pi ultimately can be rewritten as s 1 cycle s 2 cycle up to s t.



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### Cayley Theorem proof

- For a finite group  $G = \{g_1 = e, g_2, g_3, \dots, g_n\}$
- Define a map to symmetry  $\Pi_g$  defined as

$$\pi_g = \begin{pmatrix} g_1 & g_2 & \cdots & g_n \\ g_1g & g_2g & \cdots & g_ng \end{pmatrix}$$

- Show that  $\Pi_g$  is isomorphic to G and hence G is a subgroup of the symmetry group of degree n.

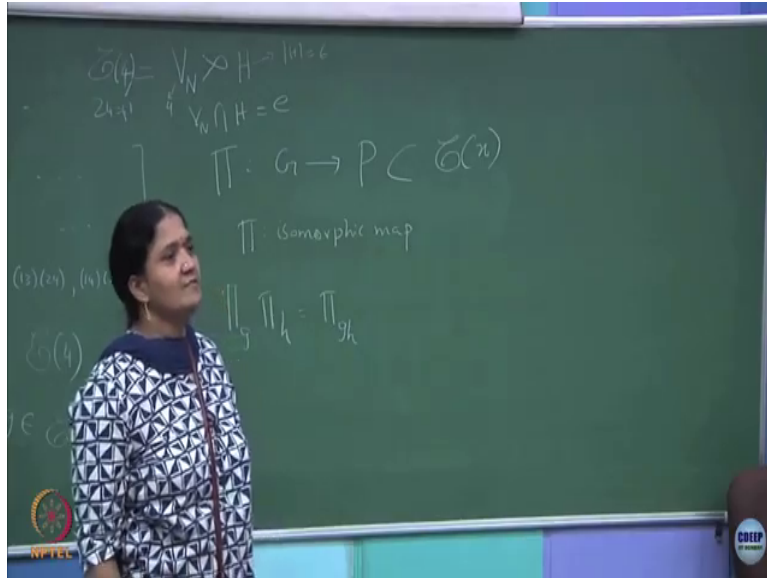



So, the next thing which I wanted to show was the proof of the Cayley's Theorem that was also one of the problems which I had given you. So, take a finite group; take a finite group. So, let us take a finite group we will always have an identity element let me call that as g 1 ok, and then let us take the order of this group to be n. Cayley Theorem says that any finite group will be isomorphic to a sub group of symmetric group of degree a, ok. So, what we will



do is we will take these  $n$  elements to be the  $n$  objects in the permutation group, in the symmetry group, and we defined a map.

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So, we are going to define a map  $\pi$ , which takes  $G$  to let me call it as a permutation group, which is a subgroup of symmetry group of degree  $n$ , ok. This is what do you want to show that, and then we want to show that  $\pi$  is an isomorphism, if you can show this then you have proved Cayley Theorem.

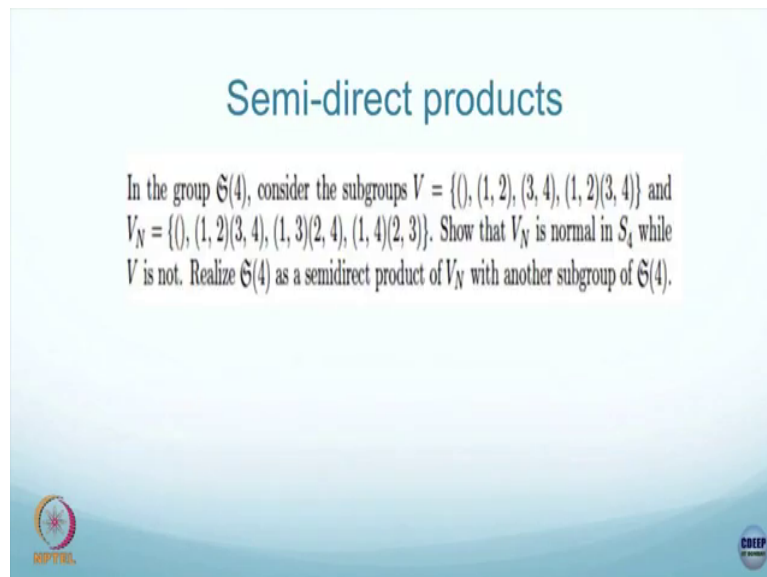
So, I have defined for you a  $\pi$  subscript  $g$  by definition, is take the set of all the elements in that group  $G$  to be the objects in the permutation group, which is getting permuted. If you multiply  $g_1$  with  $g_2$  you will get some element which belongs to the same set you all agreed right that is the definition of the group. So, I am defining  $\pi(g)$  to be  $g$  1 times  $g$ ,  $g$  2 times  $g$  and

so on. Now, I will leave it to you to do  $\pi g^{-1}$ ,  $\pi g^2$  or  $\pi$  you know  $\pi g$ ,  $\pi h$  and show that to be  $\pi g h$  these things I want you to check.

So, these are the properties to show that, this is a having a homomorphics map or in fact its isomorphic map, right. And once I show this subset of elements subset of permutation in your symmetric group of degree  $n$  will have all the group properties and it is going to be isomorphic to your finite group of degree  $n$  sorry order  $n$ , ok. So, that is the Cayley Theorem and this I gave it in one of your assignment to check and this is the way to prove it.



So, I have said show that  $\pi g$  is isomorphic to  $g$  and hence  $g$  is a subgroup of the symmetric group of degree  $n$ . This I have not shown it for you, but you can do it systematically right  $\pi h$  and then write the combinations and show that this property satisfied. What is the inverse operation, it is well defined for a permutation elements.

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**Semi-direct products**

In the group  $\mathfrak{S}(4)$ , consider the subgroups  $V = \{(), (1, 2), (3, 4), (1, 2)(3, 4)\}$  and  $V_N = \{(), (1, 2)(3, 4), (1, 3)(2, 4), (1, 4)(2, 3)\}$ . Show that  $V_N$  is normal in  $S_4$  while  $V$  is not. Realize  $\mathfrak{S}(4)$  as a semidirect product of  $V_N$  with another subgroup of  $\mathfrak{S}(4)$ .

So, the other question which I had asked, so, there was a typo this should not be  $S_4$  it should be symmetric group of degree 4, just correct it. So, every symmetry group for example, we are taking a symmetric group of degree for 4, 4 objects. I have given two subgroups.

One subgroup is where you take 1 2 cycle and the 3 4 cycle and you can write  $V$  involving it should form a subgroup which means with just with 1 2 and 3 4 it would not be enough, right, why? The set should be if you write the  $V$  as identity 1 2 3 4 is this a group sort of group because it is inverse 1 2 square is identity it's 3 4 squares is identity, but I should also allow property where, I multiply arbitrary elements and it should be in the set, that would not happen. So, you will have 1 2 3 4 anything else, this square is also identity.

So, this is definitely a subgroup of your symmetry group of degree 4 right, but is it an invariance sub group if it invariance subgroup, what do we have to show? If you take 1 2 element and a  $g$ , and a  $g$  inverse what did you get has to be some elements from the set ok, I am not even saying. So, let me called that element as some element  $H$  which is an element of  $V$  for all  $g$ , which is an element of symmetry group of degree 4. This happens then you will call  $V$  as a invariant called subgroup, ok.

So, you have to check, but I am trying to tell you that if you do this you will find that this is not same as this is not satisfied, ok. So, which means  $V$  is not an invariant subgroup is that clear  $V$  is not an invariance subgroup.

So, you need to look at the other group which is given also do a similar exercise  $V_N$  and you can show that  $V_N$  is normal while  $V$  is not. The same argument you have to do, but you will be able to show for the other group for  $V_N$ , it will be  $V_N$  will be  $V_N$  invariance. By the way  $V_N$  belongs to alternating group or no;  $V_N$  has what elements 1 2 3 4, 1 3 2 4 and 1 4 2 3 this has what, it has two transpositions every element in this group has even number of transposition. So, it will belong to the alternating group, clear. And you I leave it to you to check that this one will be an invariance subgroup which means it will be equal to, ok.

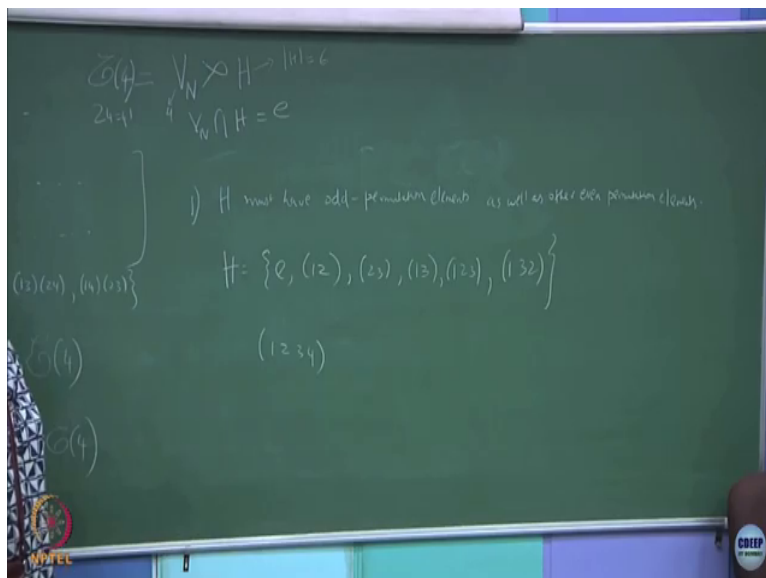
So, given this fact I have asked one more question here. Realize, see if you remember the definition of a semi direct product you will find a subgroup whose intersection with the invariance subgroup is only identity element, right, that is the definition of a semi direct product group. So, you find so, invariance subgroup was  $V \times N$  and you need to find a semi direct product with some subgroup let me call it as  $H$  and that I want to write it as a symmetry group of degree  $n$  or degree 4 in this particular example, right.

Did you people to try it out anybody has some insight on what should be that subgroup elements. What is the requirement, the elements of  $V \times N$  intersection elements of  $H$  has to be only identity element that is the definition of a semi direct product, semi direct product is given by this symbol, ok.

So, this is a symbol for semi direct product with this condition then you are asked to find a subgroup  $H$  or another subgroup such that the semi direct product gives you all the elements of that symmetry group of degree 4. How many elements are there? First check, 24 elements which is 4 factor, here there are 4 elements; how many elements should be here, semi direct product orders. What is the order of a semi direct product, if you take  $g_1$  and  $g_2$  if you do direct product. What is the order multiplicate, what happens to the semi direct product, it will also be multiplicate, what it is the change right that will also be a multiplicative.

So, which means this group should have order is equal to 6 that is the first thing, right and then you figure it out what are the elements which you can write, ok. Other thing is it is a symmetry group of degree 4, it has even permutations odd permutations,  $V \times N$  has only even permutation. So, which forces you to have at least some elements which are odd permutations such that one odd multiplied with even will give you other odd elements right. But, you should also get other even elements which means you should have even elements also in the group  $H$  whose intersection with the  $V \times N$  is null except identity nothing should be there, you agree.

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So, these are the things we observe observations are H must have odd permutation elements as well as other even permutations elements, ok. So, that is the first observation we can make. So, using this let us start generating. So, let us write H to be identity let us write 1 2. If I take the 1 2 with this 1 2, 1 2 squared is identity 3 4 is generated. So, I do not need to write 3 4, is that clear. So, what I have to do is I have to generate things which are cannot be generated from here, that is 2 3 under what else.

So, with this you have these 3 you also get various here from 3 4, 2 4, 2 3, ok. So, that is one which you can kind of guess. I should also remember I should not exceed six I should also make sure that this forms a group, right. So, forming a group means what, product of these transpositions should also belong to the set, right 1 2, 1 3 will be product of two transposition we will give you a 3 cycle right and completely you know it does like the symmetry group of degree 3, 1 3 2.

By now all of you should be comfortable with the cycle structure notation or the notation. The intersection of this with this is only identity element, I am not still shown whether it will generate all the elements, but you can check in random can you get a four cycle out of this, ok. So, I leave it to you to check if you want to get 1 2 3 4, you have to put pick one element from here, pick one element from there such that the product will give you 1 2 3 4, ok.

So, just check in random and see whether you can also generate the, you have to get all the 24 elements. This is definitely a subgroup symmetry group of degree 3 is a subgroup of symmetric group of degree 4 where you do not touch the 4th object, right. You do not need to permute the 4th object, 4th object can just remain itself a new permute only the three objects, but what I want to you to H check this at the semi direct product. We will give you all the 24 elements for this particular case and this is the way one should go about reasoning it.