Symmetry and Group Theory
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Lecture No.8
Matrix Representation: The Way Ahead

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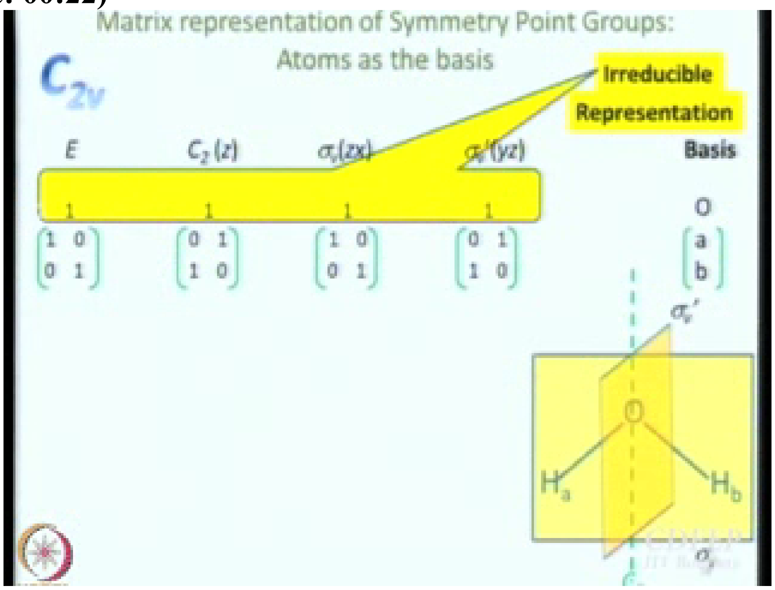

Let us work with the atom and of course the most famous C2v molecule is water we talked about water ok. The symmetry operations are the same but let us use this O and oxygen atom and the hydrogen atom as the basis. Now the hydrogen atom do not really have a and b written on them but then we have to write a matrix right. If I write H and H then it will be very confusing so let me used labels a and b. Let us begin for a while let us make out between red colour hydrogen atom and the blue colour Hydrogen atom and you have just written a and b.

What will be the matrix for E for this basis; no matter what the basis is matrix for E remains the identity matrix right. And in this case also we have the bases that is 3 dimensional so here also you have 100 010 001ok, what about C2 what happens in C2, O remains O, or it is better O remains O for everything is it not. No matter what we do is there oxygen becomes hydrogen either it is not a symmetry operation or you are a wizard of nuclear transportation ok.

Since you are not, oxygen is better remain oxygen fine now what happens to a and b they get interchange you can write the matrix now 100 what will be the second line 001 right see what has happened we have gone half diagonal one has gone half diagonal right why because a as become b and b has become a what is the third one 001 no 010 010 a and b are interchanged convince yourself that this is the correct matrix are you will convince good.

Now what about Sigma zx? Sigma zx should have the same matrix as E right same 100 010 001 right what about Sigma v dash yz again O remains the same a and b interchange positions so the matrix will actually be same as C2 right. So, now can you say what factor it is what kind of block factor which we should do, where should we draw the lines, remember all the 4 matrices has to be split exactly in the same way. How and where will you draw the line I know the horizontal line and vertical line but where?

First row first column after first row after first column this now look at the blocks may be remove 0 and look at the blocks, so it is 1 by 1 block and we have a 2 by 2 block the thing is when we talk about classes we talk about Irreducible representation only ok right now I do not know this point that I actually know that the second one is there reducible representation but then officially in this class we do not know whether the second one is reducible or irreducible. If it is reducible then the question of class does not arise right.

These are all blocks do you all agree these is how you should draw the lines right. Once again 1 by 1 matrix and we have a 2 by 2 matrix ok. We write them so now what do you have, you have two representations the first one is 1111 no matter what you do, this guys is so stubborn that is not going to change right 1111 this is therefore 1 dimensional irreducible representation ok am I sure and it is actually special kind of irreducible representation. All the characters are one which means so what is the basis here O right which means no matter what you do no matter which symmetry operation you bring in.

O does not change, O does not change means character of 1 means it is symmetry right. So, O is symmetry with respect to all the symmetry operation alright anyway the representation like this everything is one then you call it totally symmetric representation. So, 1111 or 1111or 11111 whatever it is if all the characters are 1 all the numbers are 1 now let us say that then that is called that totally symmetric representation the basis of this representation is symmetric with respect to all the symmetry operation that you use ok of course it does not mix with anything else that also is an issue that is an one dimensional representation are you ok with this ok with the block factorization ok with the concept of this totally symmetric representation, sure maybe I move on fine so, moving on.

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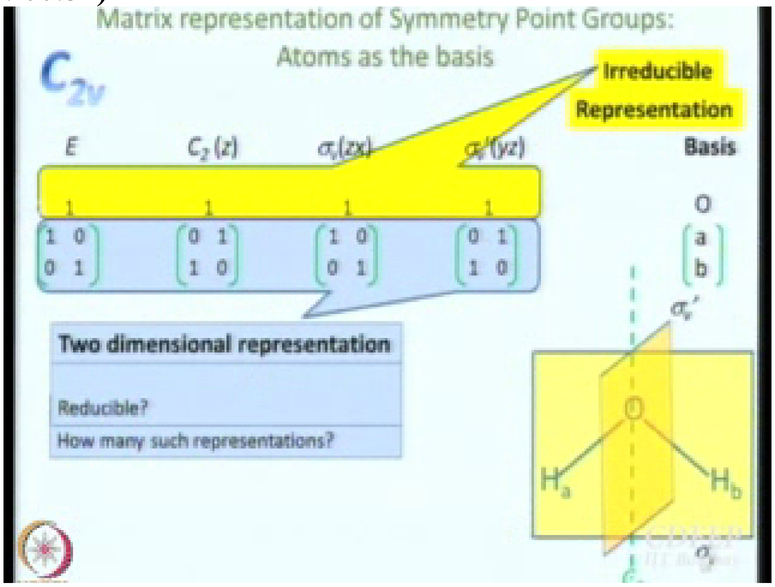

We have to think about this one it is a 2 dimensional representation right. Is this irreducible representation the question that I am essentially asking is this are this 2 by 2 matrices diagonalizable or not this is diagonalized these two are not. How does one know that a diagonalizable matrix one way of doing is similarity transformation is it not? But then it is all not easily done ok you still try to do and find whether it is diagonalizable or not. So, this is first question ok at this point without doing anything else I do not know reducible or irreducible. With benefit of my insight that it is reducible that is a reducible.

But prime of facie looking at this it is not easy to tell that whether it is reducible or not ok. The second question is that comes to as that time is that totally how many such irreducible representations are there. How many reducible representations can be there for any symmetry point groups how many reducible representations I am asking a general question for any symmetry point group what will be the total number of reducible representation.

Reducible representation yeah first many then realisation downs the correct answer that comes in is infinite. I can take reducible representation and I can combine them in whatever way I want. I can keep on increasing the number of elements in the basis right. If I am all the time in the world I can generate endless number of reducible representation ok that is infinite. But what about the number of irreducible representation actually I should have written irreducible representation here.

How many irreducible representations are there is that finite is that infinite can we determined what it is? Answer is yes, it is finite and answer is yes we can determine how many symmetry irreducible representations there are ok. But how do you know that, doing similarity transformation over and over again for everything that is not such a nice things to do. So, that comes from called great orthogonality theorem. And great orthogonality theorem arises out of group theoretical treatment of this problem of the symmetry operations that is what we are going to learn in the next few classes' right.

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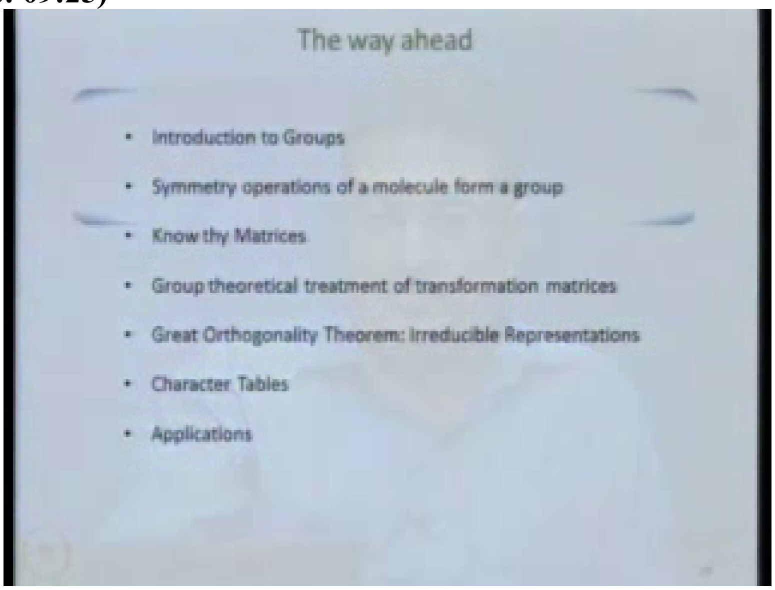

So, the plan of the thing first of all I am sure many of them know what are groups are and I am sure that many of them are lastly on this ok. So, but then if I say that I do not learn anything but nobody will be tell me anything so let us try to learn this together ok. Learn and recapitulate whatever first let us introduce ourselves to what are groups second let us come convince ourselves that symmetry operations of a molecule or a often symmetry species actually form a group ok that is where group theory works because symmetry operations in a symmetry point group actually form what is called mathematically a group ok.

This is not the seniority group junior group high security group low security group not like that this is group as defined mathematically ok fine next. Is that if you have to do that then you better know little bit of matrices once again everybody where studied but old people like me I have forgotten. So, let us remind ourselves that also, I know little bit of matrices how to diagonalise matrix, what is the matrix eigenvalue equation. How what is the unitary matrix, what is hermitian matrix.

Please do not get scared hearing unitary and hermitian these are nothing but we can handle we will do it slowly and we will learn it together right. And then that will prepare us for this group theoretical treatment of transformation matrices fine. Hence we reach our primary goal the great orthogonality theorem and as we will see the great orthogonality theorem will tell us; will answer all the questions that we will have. How many irreducible representations are there what is the dimensionality of each of these representations and then finally what are this representation.

Everything we can work out once you have mastered enough courage and crossed this activation barrier force to you by group theory and matrices ok. And it will take us may be little more than a week to get here ok. From there we workout the character tables as promised and then what we will do is after that we are back in chemistry. For the rest of the semester we start talking about applications in chemistry we will talk about molecular orbital theory before that something called symmetry adapted linear combination and then we talk about bonding by and large. If time permits you talk about molecular vibrations right so that is plan of what we are going to do.