Symmetry and Group Theory
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Lecture No.7
More on Matrix Representation Cartesian Coordinates in C2v Point Group

Let us begin in saints we have not met for some time let us do a little bit of recap today before we begin. If you want to talk about the matrix presentation of symmetry point group eventually before that let us remind ourselves what we have done. So, that is the homework what we have seen so far.

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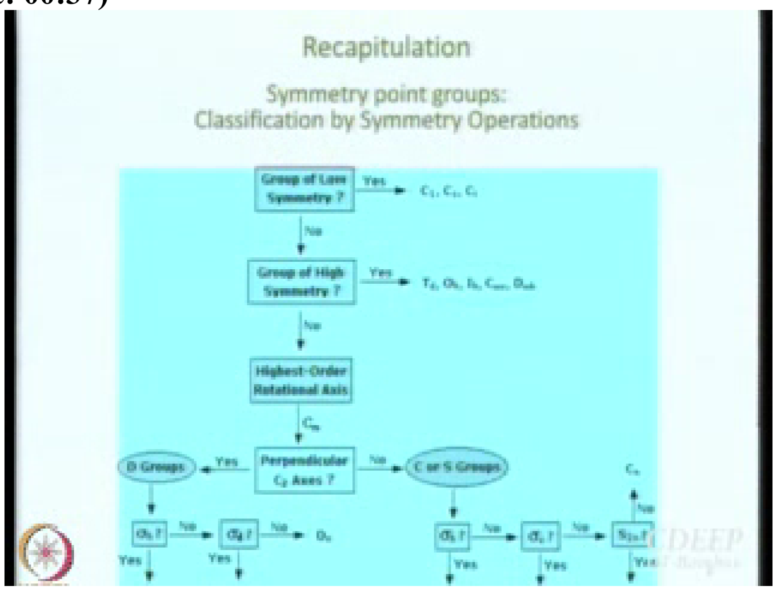

We have talked about determination of symmetry point groups using the symmetry operations that are there in a molecule and this is a flowchart that we have discussed right and we discussed that this is a flowchart that nobody needs is it not. By looking at the molecule you can figure out the only thing you have to remember is really is this CN and H2N that is what you should not forget it is little funny.

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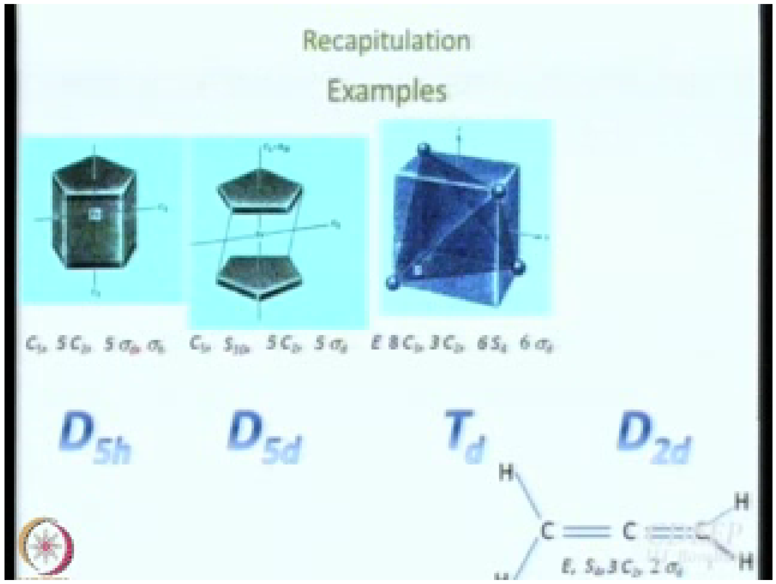

So, to start with we have discussed many examples starting with water ok some of the more notable examples of ferrocene in eclipse form and figure that it is D5h. Then ferrocene in staggered form we decided it is D5d right we talked about TD group tetrahedral group for quite some time and one thing to remember is this if you have say CH3 Cl what shape is it CH3 Cl not anymore not when you are enrolled in this course.

If it is CH4 then it is tetrahedral TD as long as you in this course CH3 Cl would mean C3v ok. So, please do not say that CH3 Cl is tetrahedral the bonds are dispersed tetrahedrally fine. But then the molecule is not tetrahedron it is C3v molecule right and ok. And then we talked about my favourite molecule that is Allene have you all; it is D2d everybody remembers Allene is D2d and then we talked substituted Allene as well.

You substitute this hydrogen and that hydrogen by 2 chlorine atom then it does not become a C1 molecule the other it becomes C2 molecule right. So, there is Allene and substituted Allene for you ok for those who came late tomorrow we are going to have the class at 6 O'clock when is your quiz? Then we have classes at 5:30, 5:30 to 6:30 we will have a concreted class that do we make up for Friday maybe or we will make up for maybe 5 minutes 10 minutes in subsequent classes or just give more homework.

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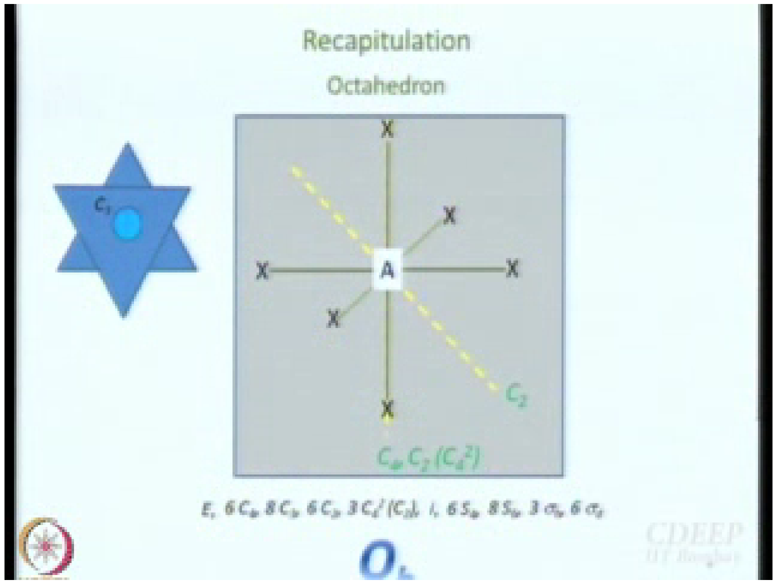

Then we talked about the octahedron and this tetrahedron, octahedron the shapes in which there are more than one principle axis of symmetry that is what make them special that is what makes them that is called platonic solids fine

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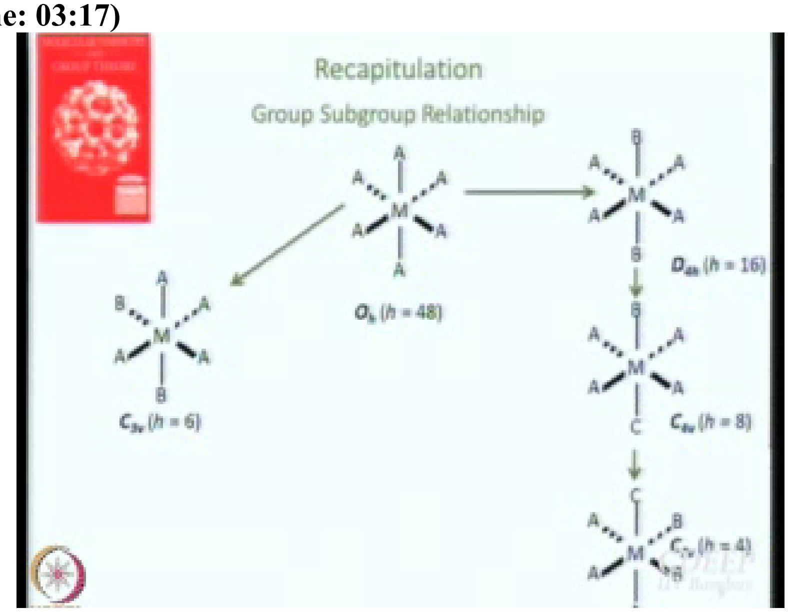

And we also talk to little bit about group subgroup relationship we are going to come back to this later on and you are going to use this big time and so far we are using that term group very loosely. But as you know group as particular meaning ok we are going to use proper meaning of group as well and then we will see how this group and subgroup become more helpful to us and then what is seems to be here. What you said is that you start with the tetrahedron and go and performing substitution on one hand you can get from OH you can get differage and C4v and then C2v which means that differage is the subgroup of OH, C4v is a subgroup of D4h as well as OH.

C2v is a subgroup of C4v D4h as well as OH on the other hand C3v is the different line of the family right it is half brother or half sister it is a subgroup of OH alright but it is nothing to do with D4h or C4v or C2v. And later on when we talk about the symmetry operations behaviour of groups and when we talk about character tables and all then we will see how this actually becomes important. And how we can simplify problems by using this group subgroup relation but that is the story for another day in future.

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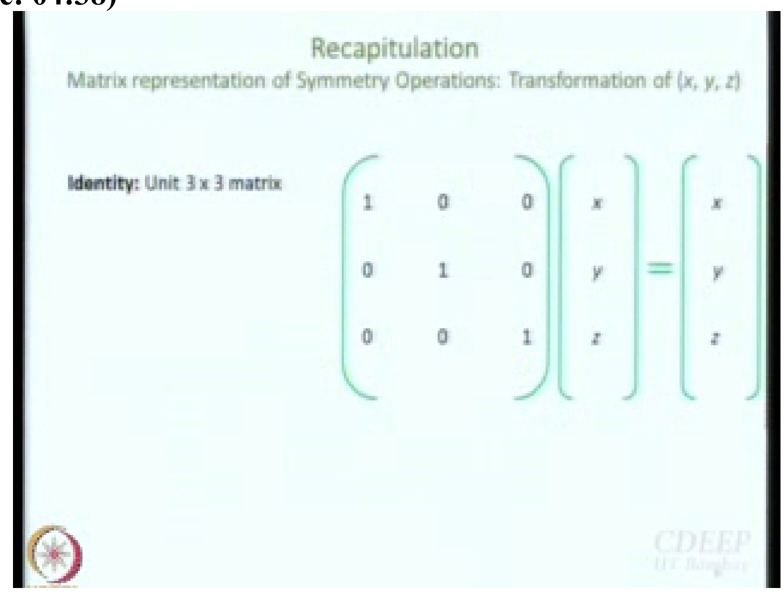

And then we have just start with talking about matrix representation of symmetry operation operations right. I think what we did is be used xyz as the basis can you close the door please and just we are started talking about how you can represent the different symmetry operations as matrices and why do you suddenly feel this urge to convert symmetry to represent symmetry operations as matrices as said do you want to translate this language into the language of algebra if this problem is to be simplified any further than this.

And way we translate using by matrices ok first we started with the easiest one for xyz what is the identity matrix, there is an identity operation that we have said, the identity matrix is your unit 3 by 3 matrix everybody will be knowing what it is 001 010 001 multiply xyz be to get xyz it is very simple.

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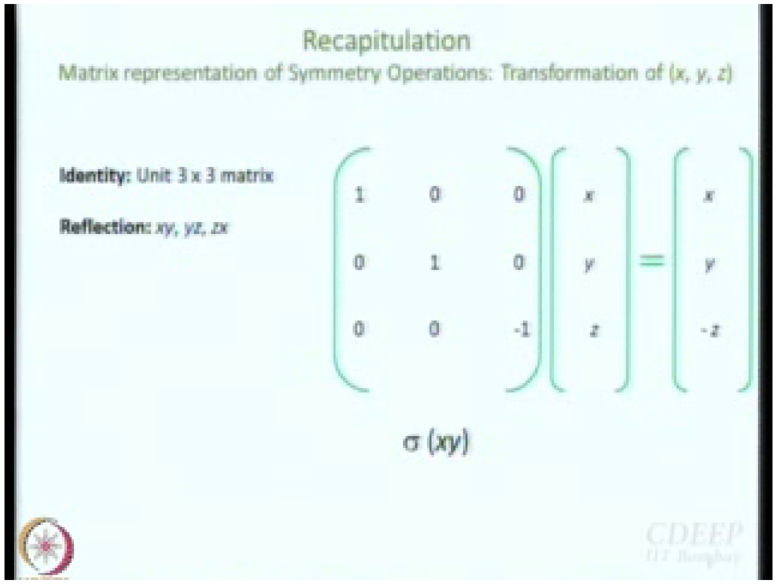

Then we talked about reflection right reflection in which plane xy yz and zx we have discussed three cases and here we all represented the xy what will happen when we reflect this respect to xy plane x and y co-ordinate remained unchanged and z will simply change sign and once again you have a diagonal matrix right all non diagonal elements are 0 and this 33 element is -1 because z changes sign upon reflection on xy ok, easy. Similarly you can figure out what are the matrices for yz and zx what will be there for zx 110 00-1 001 right.

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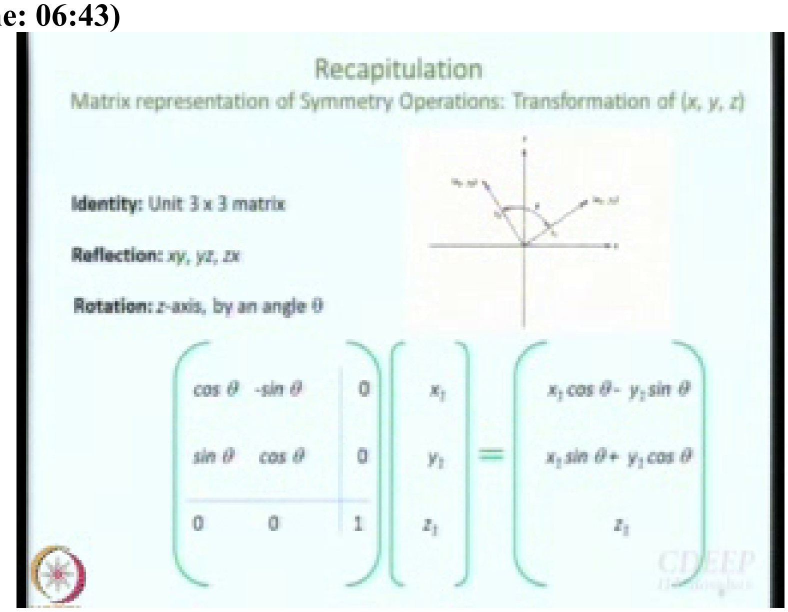

Next I think we finish with rotation and we talked about the rotation by an angle theta on the way I have drawn it here it is anticlockwise is it not. This is x1 y1, this is x2 y2 right anticlockwise and we said that the matrix that you get from that is cos theta -sin theta 0 sin theta cos theta 0 001 because x1 becomes x1 cos theta -y1 sin theta y1 becomes x1 sin theta + y1 cos theta and z1 remains z1 anyway consider this z1axis to be the rotational axis anyway ok. This is what we will work out today and just begin a little bit of variety I have given you the answer here and we are going to work out the matrix for not clockwise rotation but rather anticlockwise rotation then it is easy ok.

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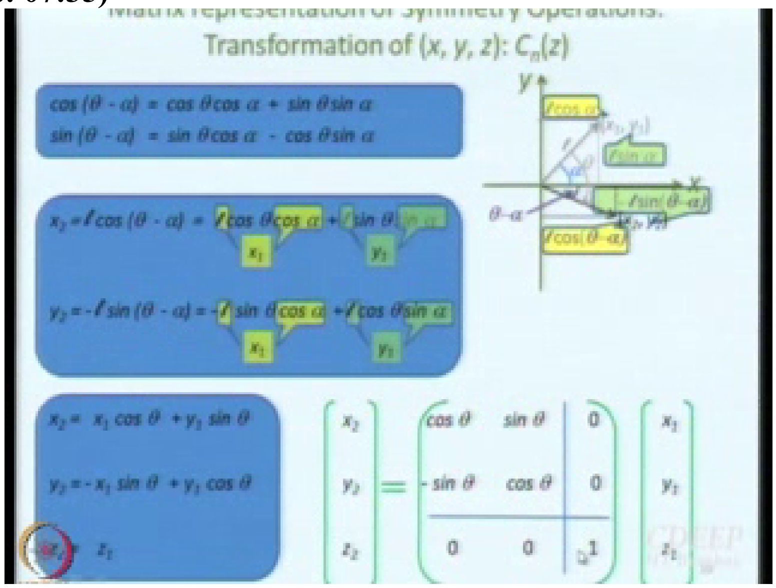

Can it is from this book Harrison Bertolucci that where it is worked out nicely but I think you do not even need the book quite simple. So, basically what we have to do it you start with this point x1 y1 ok this is what vector is this if I draw an arrow origin to x1 y1 what is it called any other name, position vector right position vector I like that name better ok. Let us say the length is l ok can you read the l there it is written in the little too stylize manner but I hope it is not too much of problem so that length is l.

Now let us say if I rotate it by an angle theta in clockwise direction theta will the length of the position vector change? No that will still remain x is it not. But let us say the new coordinates are x2 y2 ok so what is the relationship between x1 y1 and x2 y2 they are going to be related by your length l and the angle theta ok that is what will help us like x2 y2 in terms of x1 y1 and the easiest thing on the easiest way you can do this by considering the x component and y component of the position vector is as simple as that ok, if you want to do this we need one more angle and that is the angle between the position vector l the original one for x1 y1 and either x-axis or y-axis.

So, let us say the angle between the position vector l and x-axis is alpha ok. What is this angle then theta-l right, now let us go ahead and x and y components, let us start with this, this is l1 cos theta do you agree, this is l1 cos theta, I do not agree it is l1 cos alpha right Alpha not theta so, I can make mistakes sometimes I can make mistakes to test whether you are awake sometimes I will make a mistake because I have made a mistake you need to correct me in either case right.

So, l1 cos alpha and what is the not l1 cos alpha sorry what is the l cos alpha there is no l1 l2 is it not, l is same l cos alpha what is l cos alpha is x1 right, x1 and what is this one l sin Alpha simple and l sin alpha is for the y component the y1 ok simple. Now if we look at the transformed point is x2 y2 then what happens, what is this? This is l cos theta - Alpha do you agree + or - l cos theta - Alpha + or - + ok that is x2 x component right.

if you have any doubt please say and then we will go slower no issues have you all convinced x component x2 And what will be the y component this time it is minus is it not -l sin theta - alpha that is your y2 ok are you all good. Now what we do I do not want theta - alpha is it not what I want to do is I want to write x2 in terms of x1 y1 and theta right. Let us see if we can do that, to do that let us recall trigonometric relationship that we that we have studied when we little children studying in class 11.

Some of us are little children even now but what did you studied in class 11 what is cos theta - alpha cos theta cos alpha + sin theta sin alpha right. And what is sin theta - alpha sin theta cos alpha - cos theta sin alpha alright do you remember what we said you studied in childhood that is going to now come turn out to be very useful ok. Now let us simplify this very simple what is your x2, x2 is l multiplied by cos theta - alpha ok, l cos theta - alpha so, what is that then l cos theta cos alpha + l sin theta sin alpha.

What about y2 what is y2, y2 is -1 sin theta - alpha what is that –l sin theta cos alpha cos theta - cos alpha right is just that you told me II term first but it does not really matter it is a matter of choice you can choose the second one to be first no issues. In the expression of x2 what is our goal what are you trying to do we are trying to express x2 in terms of x1 and y1. So, do you see x1, where is x1, this right l cos alpha do you see y1 where is y1 l sin theta l sign alpha l sin Alpha that is y1and you see x1 and y1 in the expression for y2 as well ok.

Now what we have done as we have returned x2 as x1 cos theta + y1 sin theta I have written y2 -x1 cos theta + y1 cos theta is that correct right what about is z1? z2 = z1 alright. Is this the contrast ok when you read I have put it in the boxes or it is difficult next time I should not use this dark blue I will change it before I will send it to you no issues. Now what do I want to do next I want to write it in terms of matrices ok something like this x2 y2 z2 equal to sum matrix multiplied by x1 y1 and z1that is why I want to do ok. Tell me now what will be the matrix be very simple cos theta sin theta 0 then cos theta 0 do not say it so fast computer poor computer is not able to catch up with at your speed.

Then 001 ok that is the transformation matrix for rotation by theta with respect to z axis in clockwise direction ok, similarly the anticlockwise is something you have to work out in similar manner there is no difference really. So, now see it is block factorisable I can divided into two blocks, now dividing into blocks means I want to draw this line since in such a way and I will leave all the 0's out ok.

So, that is why I have drawn a line like this and vertical line like this so that I have one block that is 2 by 2 and I have one block that is 1 by 1 of course means only 1 number right and then all the 0's which nobody needs they are left outside the block ok. So, block factor of this matrix in A 2 by 2 and A 1 by 1 block. Before going further I like to draw your attention to something. Last day and today we have written down two matrixes both for rotation by some angle theta one in clockwise direction and one in anti clock wise direction ok.

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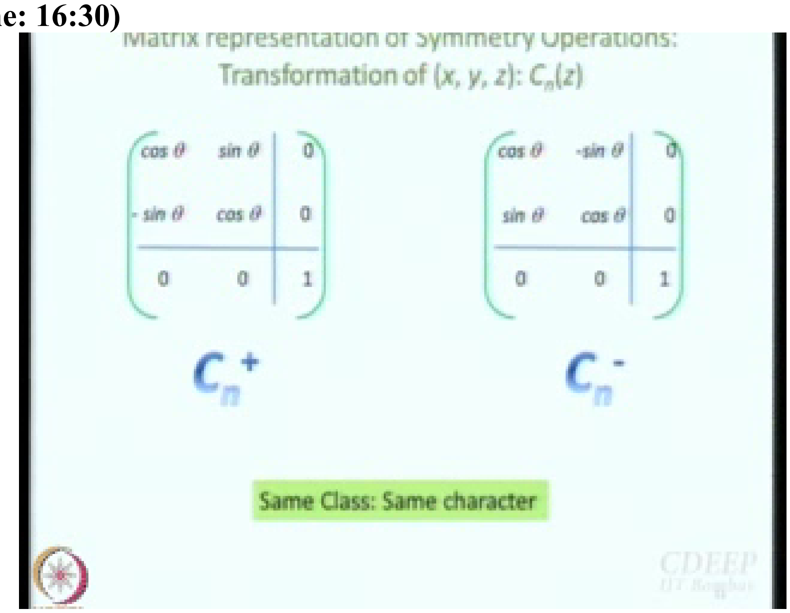

These are the matrices this is what I think I have written in the previous day right for Cn -, minus means anticlockwise and this is work, you work not right now Cn + ok now what is the similarity and difference between them first is that it is both are block factors 2 by 2 and 1 by 1 block ok and the 1 by 1 block the number that is just 1 because z does not change the line ok, why is this 2 by 2 because by operation of the rotation by theta we are essentially mixing x and y. When you mix two coordinates then you will get non-zero non diagonal elements that is point number 1.

You get 0 non diagonal elements then the coordinates do not mix with each other unsocial coordinates they keep to themselves really they here remain what they where or at most they change sign. Then you get a situation like this ok. But when you have not non 0 non diagonal elements it means is that so let us think of this block of 2 by 2 matrixes. This matrix works on what x1 y1 and gives you x2 y2 ok. Why is it that you have a sin theta here and -sin theta here you cannot write x2 in terms of x1 you also need y1 is it not.

You are mixing of coordinates ok Bala fine first point number 1 non zero non diagonal element will come when there is a there is a mixing of coordinates and point number 2 here if you look at these 2 by 2 blocks what is the similarity what is the difference. The difference is that position of the sign position and the minus sign is it not, yes they are transposed but what is same is the character 2 cos theta here also so it is 2 cos theta. So, it does not matter if I rotate in clockwise or anticlockwise direction the character remains the same.
Because what is the character carrying because the information that the character gives you, character is that trace sorry trace this some other i, aii ok. So, in this case it is cos theta + cos theta in this case also cos theta + cos theta the diagonal just form the diagonal elements there is a character right. Character does not change right it is 2 cos theta in both the cases, so the point I am trying to make is that when you do the operations on the same class then they are the same character.

CN + and CN- belong to the same class just rotating the this way or the other right same axis it will it belongs to the same class see they are having characters. This the point we will come back to later on once again you have a little more insight to character tables. So, the other point of course comes out of the characters can tell us a story ok, characters being in variant that is why they are called as characters fine.

Now so you have already learnt how to write down what are called the matrix notation for the symmetry operation ok, now we are you are going to use these matrices to generate what are called representations of symmetry point group. And in the generic representation what we essentially do is that we look at all the matrices together ok. So, what the representation does is that it tells us property of the symmetry point group or it tells us about property of certain species in the symmetry point group.

Which undergo a set of changes a specified set of changes upon all symmetry operations? So, let us see what that means. Let us work with the simplest point group that are well that will not be simplest but very familiar point group that dealt with C2v. What is the example of C2v that we have discussed water to start with what about CH2 CL2 that is also C2 is it not so many others?

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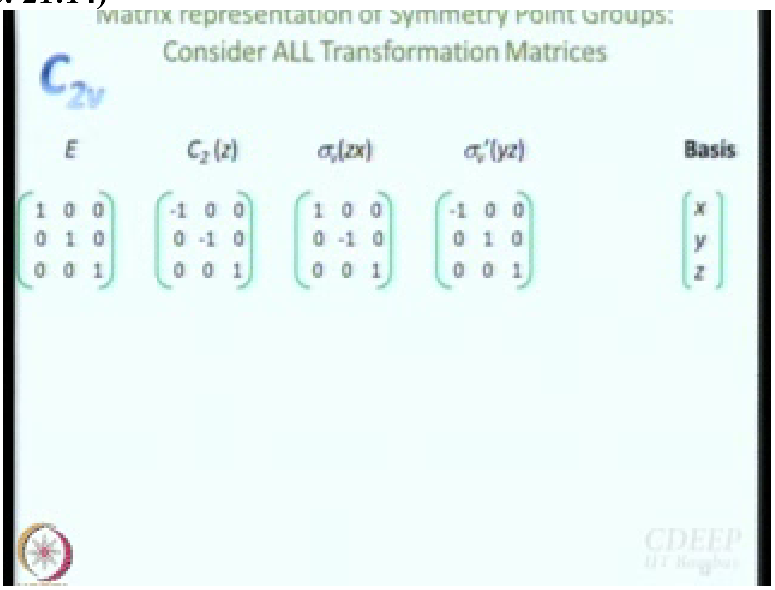

So, if you talk about C2v what we will do it is there symmetry operations of the C2v by now we know this E C2 and we considered z-axis to be the C2 axis as usual z axis is always not always most of the time designated as the principle axis of symmetry Sigma v will be there zx and yz right. Sigma v as to contain the principle axis sigma v is denoted as zx Sigma v dash is denoted as yz ok. We will take this and we are going to use xyz as basis, what is the meaning of basis I perhaps go with more general definition, basis is a collection of elements and of course elements are i mean Nickel, Cadmium and all that.

Basis is a collection of functions on which the operators are operate, it sounds a kind of silly but it is general is it not. So, this is the set of function on which our; I am going to make the transformation matrices operate and then see what happens ok fine. So, for this basis let us cancel the symmetry operation what will be the matrix for E very simple 1010 001 because identity as to be unit matrix no issues. What about C2v, what happens when I apply C2 z what happens to x, x coordinates x become -x do you agree with that x becomes –x.

What about y becomes -y what about z, z remains in variant so what will be the matrix be -100 0-10 001 ok. So, see rotation by 180 degrees is a special case of rotation by theta what you said immediately before is that when you rotate by an angle theta then you have mixing of x and y not if you rotate by 180 degrees because you rotated in such a way x has become- x. So, once again we have answered such coordinates that do not talk do not mix with each other that is why once again we have nice diagonalized matrices.

There is no non zero non diagonal elements here right because rotation by 180 degrees is such that take a vector and you just make it negative it does not makes the other one ok. So, once again unlike what we have did it in earlier we do not get non zero non diagonal element there is no mixing ok so far so good is there is a question please ask please feel free to ask question that you might think or not so intelligent questions also sometimes those are the better questions fine. Now we move on Sigma zx, z and x are on the plane they are not going to change sign what about y, y becomes -y what is the matrix 100 0-10 001 alright.

Once again no mixing why because we are taking zx now think for a minute what could happen instead zx we have to take a plane is is half way between x and y axis goes through z right but does not go through one of the axis this is your z-axis not a very good example of z axis this is z axis you are saying zx right, this is zy what did the plane was somewhere in 45 degrees is between your x and y plane what would happen then x and y would interchange right that is the other end of the spectrum.

Not only mixing not only mixing complete transformation x become y and y becomes x what would be the matrix in that case 010 100 001, so what would be the so now back to your blocks of 2 2 by 2 and 1 by 1 in that case also right 01 10 this block whatever happened is that diagonal elements are 0 non diagonal elements are 11,so if I want to work out the character what will be the character 0. So, this non diagonal element contribute to the character is it not the character becomes 0 in that case. Once again it is a kind of an extreme case of mixing where the original co-ordinate does not have any co-ordinate in the transform co-ordinate at all ok fine.

Then sigma y dash yz it is very easy now y and z will not change sign, x will change sign then what it will be -100 010 001 right. So, what I am saying is that these 4 matrices forms a matrix representation a symmetry point group C2v ok that is only the beginning not the end. Because if you look closer you can conveniently break up the matrix into 3, 1 by 1 block is it not. See all these half diagonal elements are zero is it not. It may contribute do not contribute anything, so what myself will do is I might as well do not try them write only the non zero element ok alright. Write down little nicely then of course these brackets do not need anything any more right so what I can so is get rid of the matrix.

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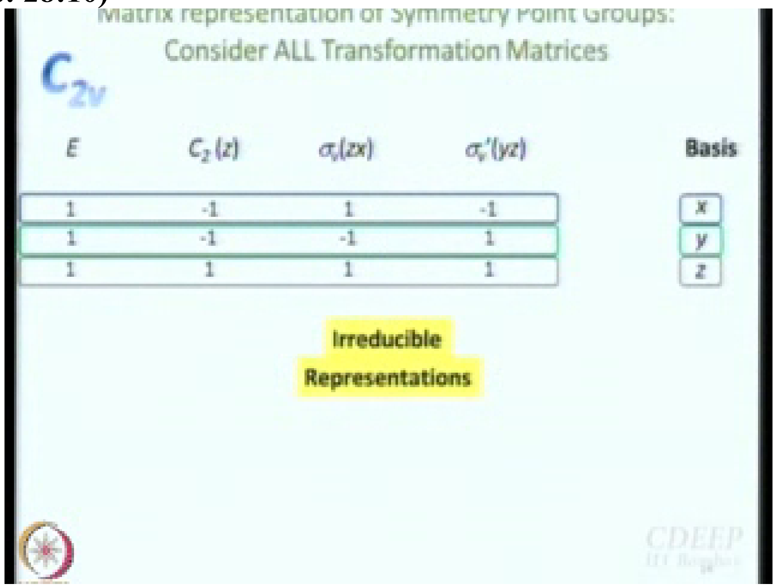

Now what do I have this 1-11-1 which is representation for x, 1-1-11 which is the representation for y 1111 is there a presentation for z ok so you have 3 different representation for the 3 coordinates xy and z ok. So, what does this tell us, look at these, what you say is that, how does the x behave x remains invariant under E, it changes sign under C2 it remains invariant under Sigma v and it changes sign open operation of Sigma v dash. So, what does this tell you about, it tells you about how x behaves with respect to all the all the symmetry operations in the point group C2v ok.

So, this a nice symmetry description of x right ok, what we have done essentially is that we are found out which symmetry species that x belongs to which symmetry series y belongs to which symmetry species z belongs we are define symmetry species alright. These are the symmetry species for you ok representation or symmetry species. So, have we at least got the resemblance of understanding what is the meaning of symmetry species right. What we see is that in this case C2v x and y and z they belong to 3 different symmetry species ok it is symmetry species or representations.

And these are Irreducible representation because you have just 11 numbers right 11y1 matrices are what we say is that the dimensionality of each of the symmetry species is 1, 1 dimensional

Irreducible representation one dimensional representation therefore it cannot be Irreducible dimensionality cannot be less than half right you cannot have half the number remember that riddle it takes 8 days for 4 men to dig a hole 2 how many days it will take for 8 men to dig a hole no actually it should be half.

How many days does it take for 2 men to dig a hole there is nothing like a half, hole right sorry I got it wrongly how holes these two men dig in one day answer is still one you do not have above one. Similarly here also you cannot have half dimensionality half does not make any sense one is the minimum number so it cannot be reduce to any further. That is why they are called Irreducible representation. Irreducible representations are also called symmetry species because they tell you how certain functions behave when subjected to each and every symmetry operation in the point group ok understood so that is what it is.

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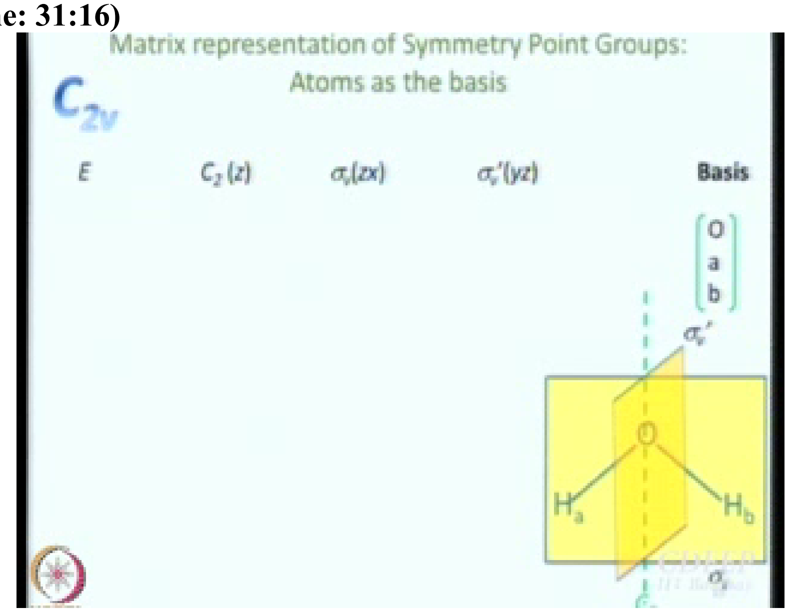

Now what we can do it let us study and change the basis and see what we get. Working with one bases is not enough work with xyz and be happy go home end course give everybody A to everybody is not a good idea right what you are doing right now is those 10 blind man trying to define an elephant somebody says of elephants looking rope and somebody says elephant looks like housewife right. So, what we should do is we should see what happens when change the basis. Let us change now maybe the basis that is more tangible to chemistry then xy and z.