Chemical Applications of Symmetry and Group Theory
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Lecture – 15

Hello everyone, hope you are doing well. So, in the last class, we learnt about the matrix algebra and today we are going to utilize those you know knowledge about matrix and matrix algebra to find the representation of point of a group in general. So, this will continue for few days. So, how to find out the representation of a group and how to utilize that, and then we will see there the different types of representation, different ways you can find the representation and all these things.

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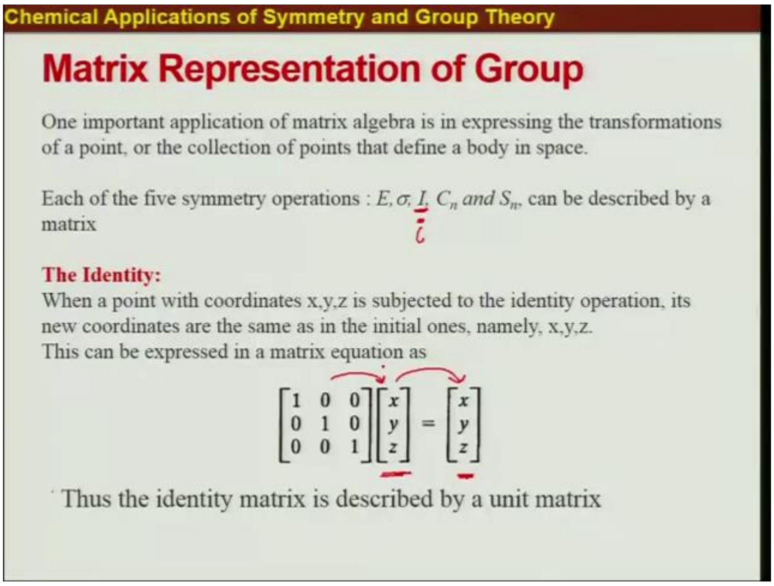

So, let us get started first you know to find out how to form a representation of any given symmetry operation. Now, one important application of matrix algebra is in expressing the transformation of any given point or the collection of points. So, it can be a single point as well as the collection of points which defines a body in space. So, we will use this particular property. So, this particular you know this you know power of ability of matrix algebra to this transformation of one particular point or collection of point in belonging to a particular body in the space. We will use this property to have a representation. Now that is what we are going to do.

So, if this matrix algebra can to that to any particular point then it is understood that you know this symmetry operations can be represented by matrix algebra, which simply to understand. Because a symmetry operation does the same, it transforms one particular point of a body to another using an indistinguishable structure. And matrix algebra also does very similar thing it takes one point and transform it to another point in the prop body. So, I should be able to express all this you know identity or you know reflection symmetry inverse. So, this should be small I here, a small correction here. And proper axis of rotation or improper axis of rotation, all this symmetry operations can be represented by matrixes and that is what we are going to do now.

So, we will start by element identity and there are following identity operation. So, in case of identity, what we have that you know we have no change as such. So, if one does nothing you say that, I have performed an identity operation. So, if there is a point in a body whose coordinates are x, y and z, after the identity operation has been done on that particular point, what is the configuration or what is the coordinate of that particular point it is x, y and z. So, in order to have it you know matrix that will resembles this transformation that is x, y, z which is normally written in terms of column vector as you can see on your screen.

So, you start with have an x, y, z column vector which you know denotes that particular point that we are considering here. And then after doing the identity operation my point becomes rather remains x, y, z which is also represented by a column vector. So, since there is no change of this particular point. So, it will remain the column vector here, and column vector having the same element in the same order. So, I need to find out a matrix which will help me going over to here. So, essentially this is nothing no changes happen. So, I should have a matrix which is capable of doing a multiplication with this column matrix or the column vector. So, I should have the same property which we discussed in the previous class.

So, it should have definitely three rows. So, if it has three rows, then it can have multiplication. And in this particular case, I should have three rows and three columns. So, the in sense I should have a 3 by 3 square matrix that can act as the identity operator and it should not change any of this x, y, z in the column vector. So, only way I can satisfied that if my matrix is this that is all the diagonal elements are unity and rest of the elements are 0, which is nothing but the identity matrixes. So, this was very easy right.

So, in order to represent an identity operations symmetry operation which can be acted upon any given point any general point whose coordinates are x, y and z that particular matrix will be an unique matrix or the identity matrix. So, very easily we can get the matrix representation for this identity operation

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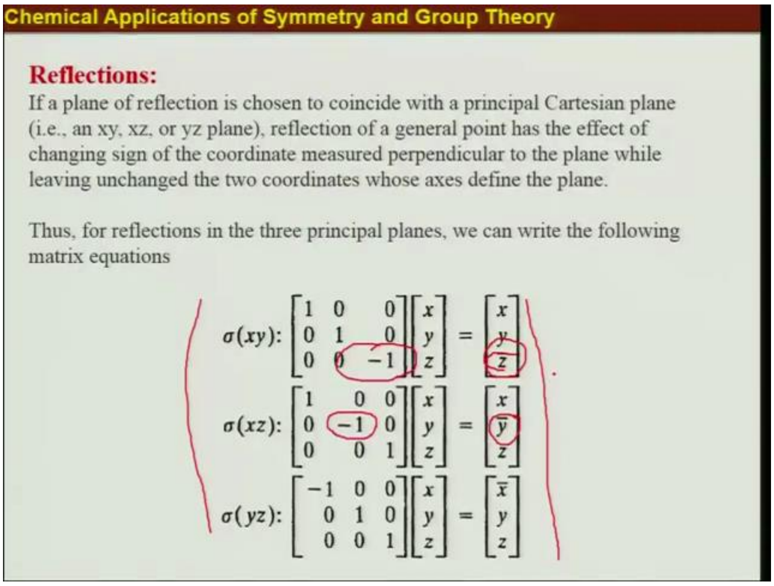

Now let us move onto other type of symmetry operation. So, we will start with reflection next. So, reflexive symmetry all of us know very well. Now if I select a plane of reflection, which coincides with the principal Cartesian plane. So, what I mean is if I have Cartesian coordinate system, so x, y and z in this Cartesian coordinate system I have a xy plane, I have xz plane I have yz plane. So, I can choose if I am given the freedom when I can choose my reflection plane of reflection to be one of this xy or xz or yz planes which natural to any Cartesian coordinate system. Then reflection of any general point has the effect of changing sign of the coordinate measure perpendicular to the plane while leaving unchanged that two coordinates whose axes define the plane. So, what does it mean?

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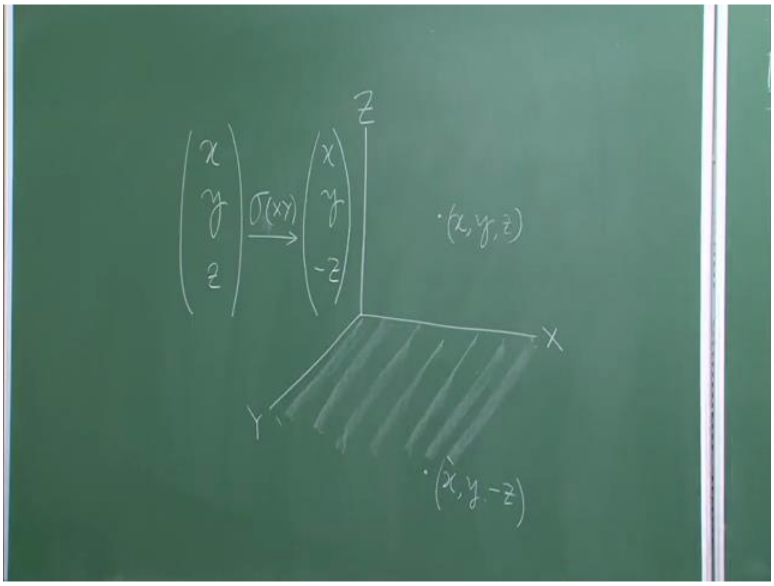

So, let me explain this by using the board. So, suppose I have my coordinate system given like this. So, this is my xz plane, and this is my xy plane and this side it is my yz plane. Now, I suppose I take any of the given planes to be my reflection plane - say for example, I take my xy plane. So, xy plane how I can depict it so, this is my xy plane this, this is my xy plane. Now, I have any general point here. So, let me say it is coordinate as x, y, z.

Now what will be the fate of this reflection operation see since I you know reflection plane coincides with one of this natural you know Cartesian coordinate plane that is xy here. So, none of this x and y coordinates will change correct because this will remain at the same place x and y, but this z which the z coordinate which is perpendicular to this plane will get reflected the other two will remain unchanged. So, after reflection, it will go somewhere below the plane. So, there this point will have coordinate x, y and z, I said it will be reflected. So, I know, right now I have the point where the z coordinate is a positive z direction correct. So, now, this z will go downside and it will have a negative coordinate. So, it will be exactly inward, because reflection will take you equal distance on the other side of the plane. So, you have minus z, so that is what we wanted to mean and you can do this for if you choose any other planes. So, if you choose say for example, xz or yz plane to be your symmetry reflection plane you can find the same thing. So, one of the coordinates will you know become negative essentially. It will change the side, but another two will remain unchanged.

So, now, we are ready to find out the of matrix form for this sigma planes. Now, hence what we will be you know talking nodes general way that is we will talking about say sigma x y sigma x z sigma y z by because we will taking any general point on the space and we will be dealing with this Cartesian coordinate C n Cartesian coordinate. So, for one particular point, I have three Cartesian coordinate system. So, we will define our symmetry operations also in terms of those x, y and z. So, very often you will get to hear that only you know c to z, c to x or you know sigma x y in that way.

So, now, one more thing I mentioned here. So, if I can write this position coordinate in terms of a column vector, what I can do I can write x, y, z correct. So, now, when I have this sigma x, y, so I will probably write it like sigma x, y if I operate on this one, what is happening x and y remaining same and z is becoming negative. So, you have x, y and minus z this is why final matrix after I operate sigma x y on this column vector. And you know if only the sign which is changing for one of the elements of this column vector and rest of them I remaining completely unchanged. So, you have to find the matrix form for this particular operation sigma x y I have to you know do something that we have to follow matrix which makes this transformation from one column vector to another column vector.

So, here if you look at on your screen, you can see the matrix representation for sigma x y and this. This will be pretty easy for you to understand since x and y they are remaining unchanged after this reflection operation. I will have the elements as one in the diagonal for say the element 1 1 and element 2 2. Now, the third one that is the 3 3 that is going to you know change the sign of the coordinate z coordinate, so that is should be a negative sign. So, it will be 1 1 minus 1 in the diagonal and obviously, the other of diagonal element will be zero because if it is if other elements has some value in I will not get back my this column vector.

So, similarly, you can figure out what will happen to the column vector, when we have a sigma plane along x z or y z planes and the corresponding matrixes from also you can easily figure out. And you can see if we compare this 3, you can see that the you know the position of that negative one is changing with respect to the you know the column vector; as we change the column vectors, this is also changing. So, you can just you know see the one to one correspondents between this position of this matrix element and the corresponding change here. So, similarly you have changing sign here for the y and accordingly your matrix will be a negative sign for this particular element here. So, it should not be very difficult for you to form any such matrixes and suppose you would have to do it for more than one points, we should be equally able to do that.

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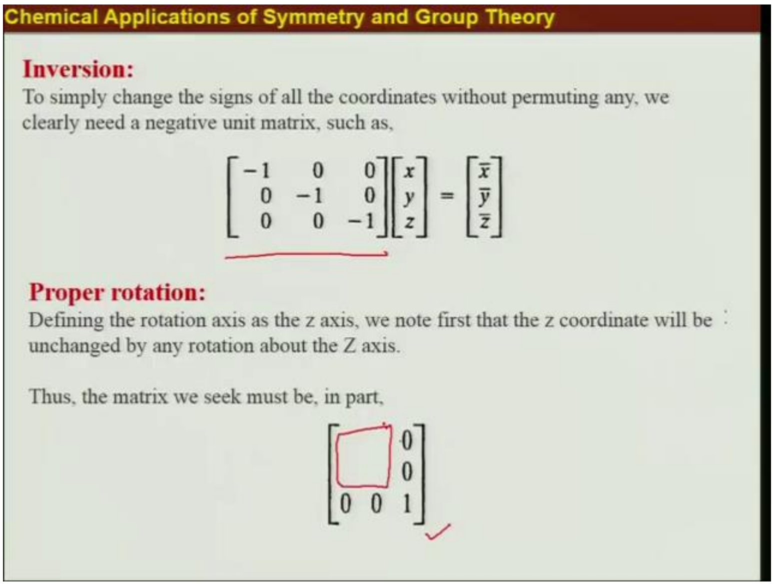

Now, let us come to inversion. Inversion is another one, which is not too difficult. In case of inversion, what do you have you take any general point on the body, if it is coordinates are x, y and z then after the operation is done that is after the inversion symmetry operation is done on this particular point each coordinates will get inverted. What does it mean that x will become minus x, z will become minus z, y will become minus y. So, you get from x, y, z column vector to minus x, minus y, minus z column vector. So, here in this minus x, minus y, minus z are represented by writing x bar, y bar, and z bar that we have come across in one of the previous lectures.

So, in order to inward the sign for each one of the column vector, but not changing you know its x character. So, like you know I am going from x to minus x, but I am not going to x to y or x to minus y. So, I mean x is remaining x, only the sign is changed. So, in that case, this will be exactly similar like the identity matrix with a negative sign. What does that mean the diagonal elements will be minus 1 minus 1 and minus 1 that is what exactly shown here. So, this is true for any representation that you can form using this three coordinates.

So, now, I said like here I have only one point. So, I have three coordinates if I would have like you know a four or five points. So, I will have three into the four or three into five such coordinates. So, you accordingly your matrix size will go up. So, for you know three coordinates, I have 3 by 3 matrix; if I would have like two points I will have total six points because I will have x 1, y 1, z 1, x 2, y 2, z 2. So, by matrix would in 6 by 6 matrix and I will have six diagonal elements which will dictate the fate of this points at the starting point to the ultimate (Refer Time: 16:22), so that is about the inversion symmetry and its makes its representation.

Now, we will look at the proper rotation. This is one of the most important and vital. So, let us look at this proper rotation, and how can we find out the matrix representation for proper rotation. Now, here also we will take a general point having the same x, y, z coordinate. And we will have another assumption that is the proper axis of rotation that we are going to tell with that is along the z-axis.

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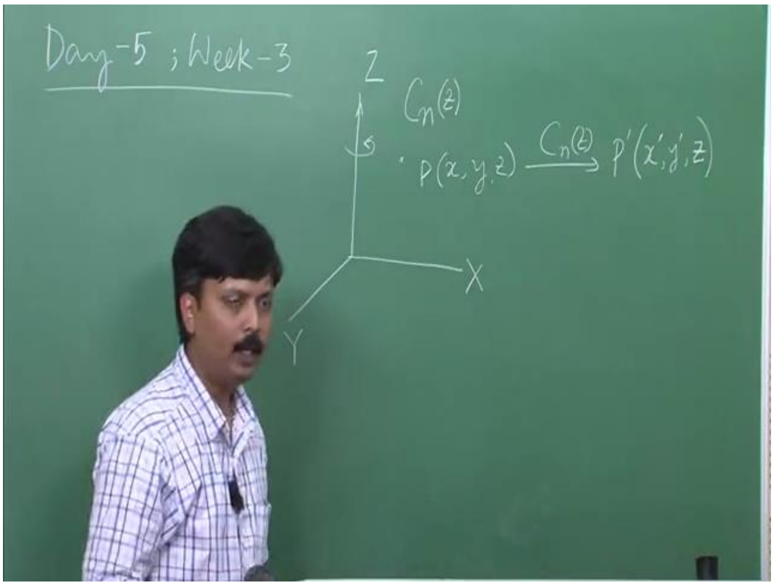

So, which means if I have same coordinate system again here sorry then my principle axis of rotation will be along about this axis. So, I will say this is I have some C n, C as C n z that is you know tell you that the C n axis is along the z coordinate of our Cartesian coordinate system, and then we will do all the operations. So, now, one thing is pretty clear from this assumption that if I take any general point here on this in the space, say I take a point here which is p having x, y and z coordinate like before then no matter what angle this C n rotates. So, suppose I included by 60 degree or 120 degree or any amount of degree, the z coordinate for this particular point is not going to change, the value of z will remains same, and it will be on the positive side of this z-axis all the time.

So, after I have operated C n z on this particular point, it will be something like you know point say P prime where this x be x prime, y be y prime, but z will remain z. So, if I have to find out the matrix, I can always say that ok, I do not know about the x and y part, but the z part will be having an element which is unity like what is shown here on the screen. So, I do not know what are the elements that are going to be here because I do not know what are my x prime and y prime, I know for sure that z remains z. So, that will you have this you know this 0 0 1 and 0 0 1 here correct that will not change prime z.

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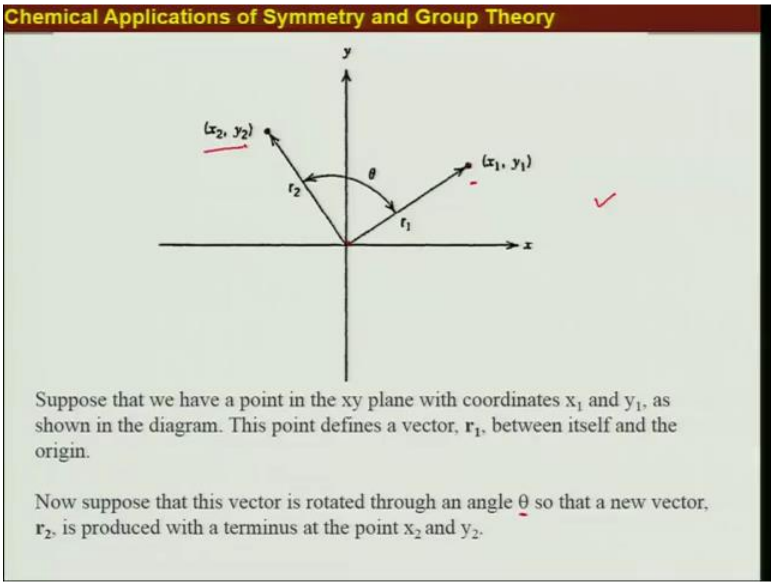

Now, we have to find out what will be the phase for x and y after I give a rotation. So, our idea will be to find out most general form of matrix representation by which I can you know I can get a matrix form for any given C n, n can be 2, 3, 4 whatever but I should be able to do that. So, let us try to do that. So, suppose we have a point in the xy plane with whose coordinates are x 1 and y 1 that is what is shown in this particular diagram. So, I have this particular point to start with. So, this point is described by a vector r 1, and this r 1 will travels the distance from this by a particular point to the origin. Now, suppose that this vector is rotated. So, I give a rotation like this and the angle of rotation is theta so that we get a new vector whose vector the corresponding radial vector is r 2 and the new points are x 2, y 2.

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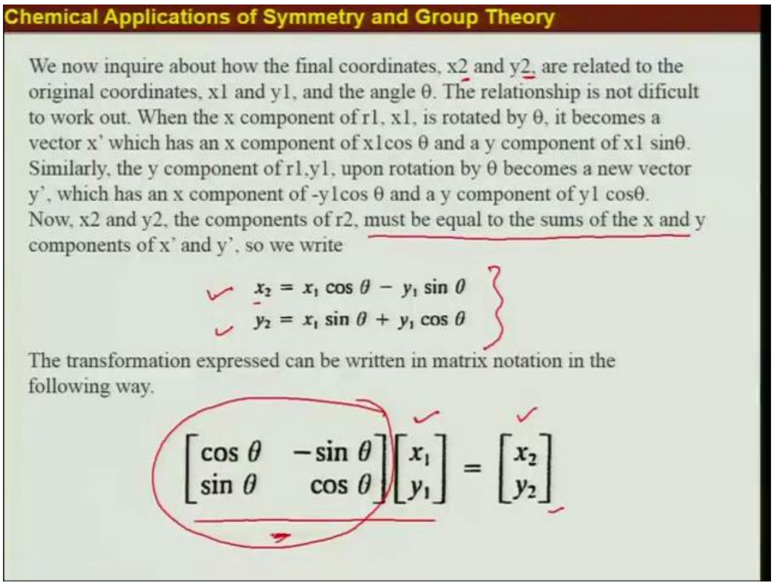

So, with that set up, we will try to enquire about how the final coordinates x 2 and y 2 are related to the original coordinates x 1 and y 1, and also the angle theta. So, we can you know work this out. So, how, so when x component of r 1 x 1 is x 1 actually this rotated by theta, it becomes a vector x prime which has an x component of x 1 cos theta and y component of x 1 sin theta. This is the simple geometry problem. So, you can easily find it out. And similarly we can have the y component of r 1 say y 1 when we rotated it by theta, it becomes new vector with new vector y prime which has an x component of minus y 1 cos theta and a y component of y 1 cos theta.

Now, x 2 and y 2 the components of r 2, which is a new vector must be equal to the this is very important right this must be the equal the sum of x and y components of this x prime and y prime. So, thereby we can write these two equations is given here, so equation 1 and equation 2. So, here one thing I will mention all this 2s are suppose to be subscripts for some reason is I mean as such. So, you can correct this one and you can write like you know this x subscript 1 or y subscript one, but that will not make any change to the context at all. Now, once you have you are written all this equation, you can find out the transformation matrix, because your aim is to find out what happens and what is this x 2, what is the y 2. Now, we have found out the x 2 in terms of x 1 y 1 and the theta and you have found out also about the y 2.

So, now, if you couple these two equations, you can very easily find out the matrix from that. So, the matrix form that you will find out, if you utilize these two equations is here. So, originally you had x 1, y 1 as your column vector, now you have x 2 y 2. And this is the matrix which you have to apply on this x 1 y 1 column vector, so that you get x 2 y 2 column vector. So, in the sense, this 2 by 2 matrix that is on your screen here that represents that you know empty space that was left where we started to forming the matrix for C n in general like we brought the value for the z coordinate transformation, but we did not get for the x and y. Now, this 2 by 2 matrix will fill that gap here.

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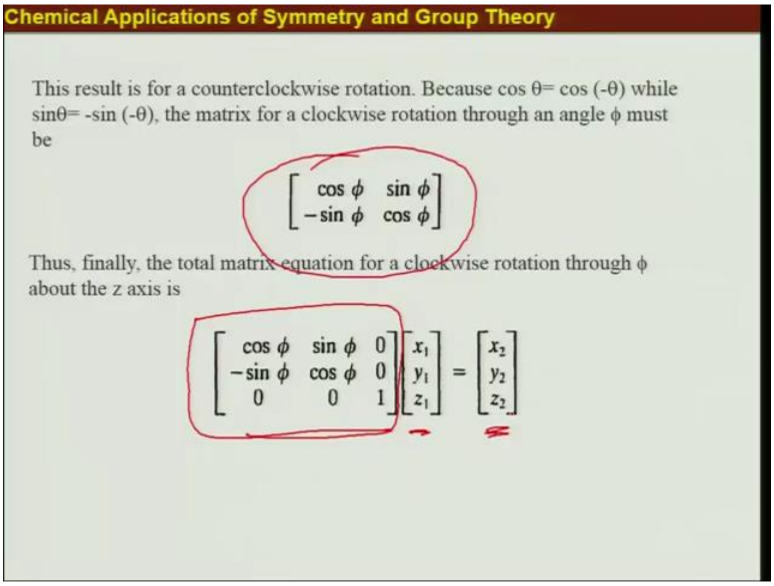

So, if we do that all together, what we get is here, now one thing one has to be very careful about what is the orientation of your rotation, it can be either clockwise or counter clockwise. So, whatever we did we rotate it in this fashion right, if we just go back here we went from x 1 y 1 to x 2 y 2 which is counter clockwise. So, all about derivation is based on so far a counterclockwise rotation. Now, if we want to do it for clockwise rotation that is very easy, because cos theta is equals to you know cos theta and cos minus theta are same while you know sin minus theta is minus sin theta. So, utilizing that we can find out the 2 by 2 matrix for a clockwise rotation as well which is shown here. Now, finally we can write the overall matrix for clockwise rotation by this expression.

Now, the beauty of this matrix in terms of this angles phi or theta whatever you use is that you just give the value of that particular angle. If it is C 6 then you give 60 degree; if it is you know C 2, you give 180 degree and you get the corresponding value for cos or sin phis and you get the matrix, alright. And that matrix will act upon this x 1, y 1, z 1 column vector and ultimately give you the final result. So, you can figure it out yourself that what will be the form of the matrix for any given C n, C 3, C 4; C 5 whatever you can think of you can try those values and get the matrix forms.

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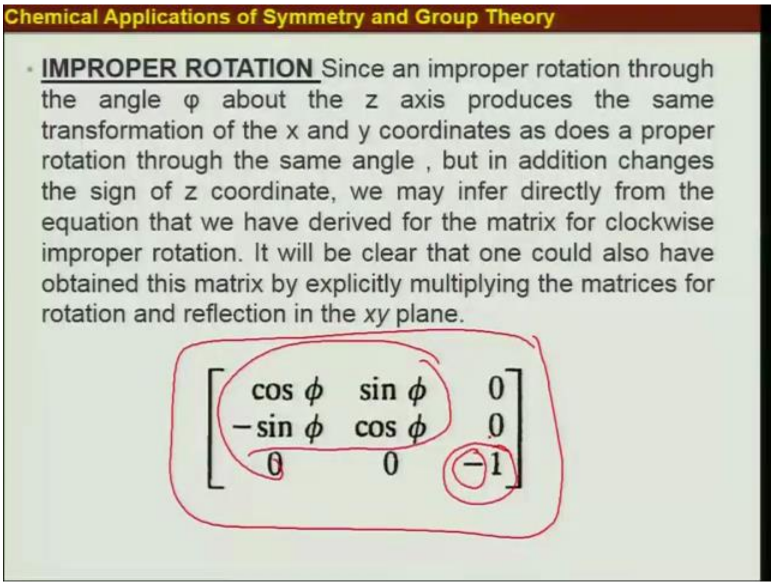

Now, we are left with the last one that is improper rotation. Now, it should be straightforward for you by now. The reason is we have learnt about the proper rotation, we have learnt about the reflection. So, improper rotation is nothing but you know rotation followed by a reflection. So, in case of proper rotation, we have a matrix like this. This is my proper rotation barring this one. So, for a second, if you think that ok there is no minus here. So, this is the matrix for my proper rotation.

Now, in case of improper rotation you rotate, so you rotate their angle and you use this matrix and get the matrix form for that one. Now, after this rotation you have to get a reflection on the perpendicular plane. So, you know exactly which is the plane. So, first you rotate around z and then you reflect around xy plane. So, whine you have sigma x, y what is that coordinate which changes is z. So, the z will be minus z correct after you get that reflection. So, you have the rotational component here, and this component with this negative sign is further reflection on xy plane and exactly that is what is the overall matrix representation of improper rotation.

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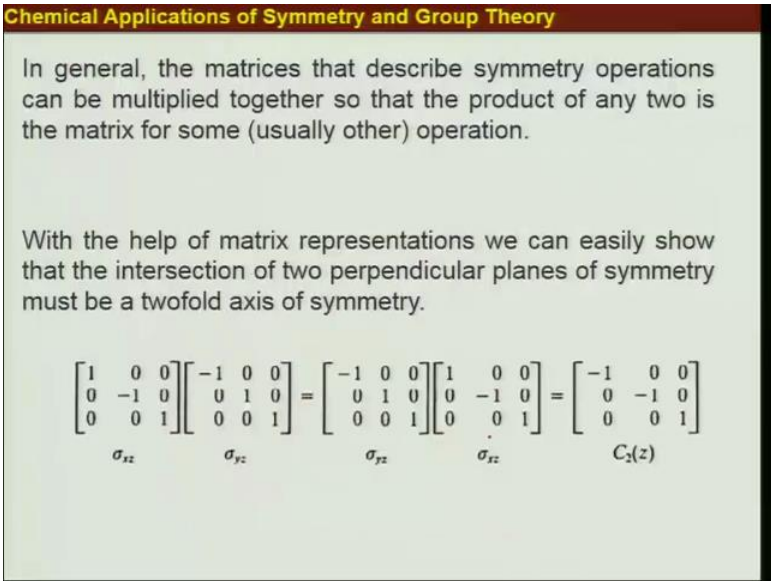

So, we can go ahead and in general we can find the matrices that describe symmetry operations, and we can verify that this matrices which are representing the symmetry operations. They are equally capable of doing the successive operations at if this you know multiplication of two matrices corresponding to two symmetry operations will generate a matrix for another symmetry operation, if suppose I have like sigma x y, sigma x z and sigma y z successively, then I am suppose to get C 2. Now, if we take the matrix forms of sigma x z and sigma y z and do the multiplication then I will end up getting a matrix representation, which actually gives the C 2 z, actually gives me the matrix representation of C 2 z.

So, this you know matrix multiplication you know can satisfy the successive operations of this symmetry operations. So, the bottom line is we see here that this symmetries algebra can very well represent the symmetry operations of any given particular molecular point proof. And we showed very generally that this hold good and you can take any specific point also and form their own matrices and verify this whole the process that we have we gone through today. So, we will stop here today. And the next week when we come back we will look at in a greater detail about the how to form the representation of a group as a whole. So, till then I will leave you with this, and I will request you to practice little bit more about the matrix how to form the matrix representation of similar symmetry operations.

So, thank you for your attention, see you next week.