Chemical Applications of Symmetry and Group Theory
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Lecture – 14

Hello and welcome to the day 4 of the third week of the lecture series. I hope it you are doing well and I also hope that you are following the solution that I have been making, like guess you have practiced lot regarding the (Refer Time: 00:36) position, if not then please do it.

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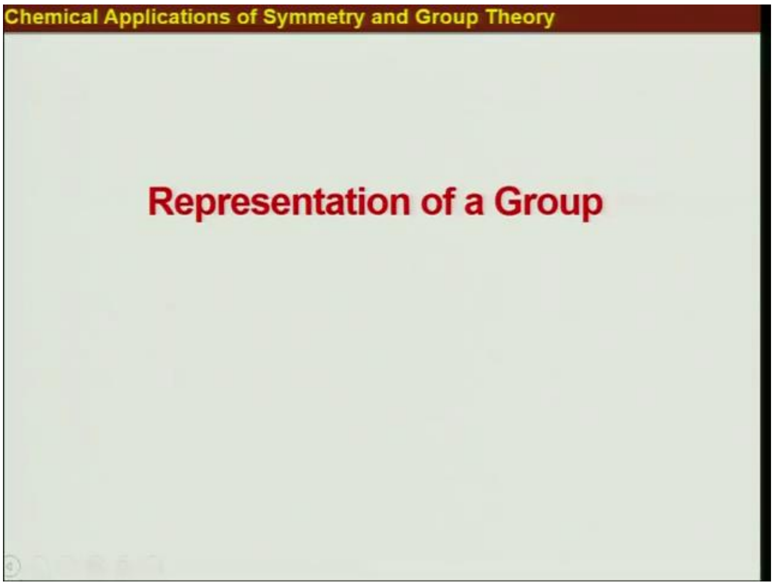

At this context I will also try to make a note, that you can consult the book by Harrison Bertulus, which was suggested originally for this stereographic position part and group multiplication table formation, you can consult any standard book on group theory. Any mathematical book and also you consult the book by Frankelbite Cotton. So, with the knowledge that we have gathered so far, we will now utilized them to form something called representation of a group. So, what do we understand when you say representation of a group? So, we have learnt to write a group in terms of the symmetry operations. So, when we particularly talk about the symmetry point groups.

Now, we write in terms say all this so implied notations like e, c n, sigma v, sigma e, sigma d, i, s n l all those things. So, that is fine, now if you have to utilized the group theory to you know understand you know, several molecular property, particularly in the context of the symmetry of the molecule, then we need to have, you know, proper mathematical representation of this symmetry operations. So, what is, you know, way to form mathematical representation of the symmetry operations? So, if you are you know familiar with, you know, quantum mechanics then you probably know that one of this, one of the ways is to utilize matrix. So, here in case of you know symmetry point groups, we will use matrices, to represent the symmetry operations and thereby we will be representing the whole group by those set of matrices that actually represent the symmetry operation.

And then we will we will use some other properties of those matrix representations, to make our life more simple and the. So, let us try to learn about this representation of a group and before we go and the form the matrices for symmetry operation and thereby the whole representation of a group in transfer matrix, we will try to learn little bit thing about matrices, Matrix Algebra. Many of you already know Matrix Algebra, but for those who does not know Matrix Algebra or have learnt some time back at once to you know, have a you know brush up, then for them we will go through the basic Matrix Algebra here. So, we will give a briefly review of Matrix Algebra.

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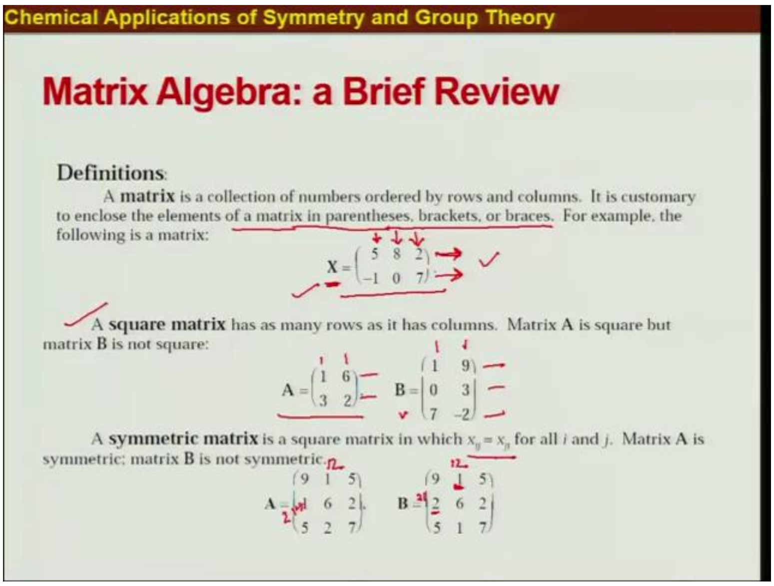

In this section, so, first we will deal with certain definitions. So, first case we have to know what is a matrix. So, if you look at your screen, the definition of matrix it is given there, which says, but a matrix is a collection of numbers ordered by rows and columns. So, if you have some numbers, some digits, which are ordered in rows and some columns. So, its array and how it is presented? It is presented in terms of you know, it is like the numbers in rows and columns they are written within parenthesis. So, that what is also mentioned here, that the element of the matrix, so, all the numbers that are there in any other rows or columns, they called element of matrix. So, all this elements will be in parentheses, brackets or braces.

So, an example is shown here, where this X which is written in bold term. So, normally when you know use a symbol for any matrix, then you use either a bold or you know, bold italics or some you know particular type of script. So, see this X is a matrix, which is you know within in this way. So, you can see, there are 2 columns, one here, one here, correct? And there are 3 rows, sorry, this 2 are rows, I am sorry and the here are the columns. So, I have 3 columns.

So, this matrix X has 2 rows and 3 columns. Now this is general example of matrix. Now if by any chance, a matrix has you know, n number of rows and n number of columns, that is the number of rows and numbers of columns are equal, then we call that matrix as a square matrix. Now an example of square matrix is given here, A is a square matrix, because it has 2 columns and 2 rows, so numbers of columns rows are equal. So, this A is a square matrix, while if I look at the matrix B here, it has 2 columns, but 3 rows, similar to the example shown in the top. So, this B or this X here, they are not square matrices.

Now, one more types of matrix that we can think about is a symmetric matrix. So, a symmetric matrix is a square matrix, in which x i j equals to x j i. So, this i and j are used for noting the rows and columns. So, ith row and jth column is given by x i j and the jth row and ith columns is given by x j i and x is any element. So, as whole any element is any element of a matrix is given by, if x matrix element is x, in its x i j, but i is row and j is a column. So, for all i and j if this equality holds, that x i j equal to x j I, then the matrix is called as square matrix.

So, if you look at here, the element saying one corresponding to row 1 column 1 is 9 and the you know, the element corresponding to row 1 column 2 is 1, on the other hand, if you look at the matrix B, you will see that the element for which the row 2, column 1, it is just opposite of the previous example, you know, is the same. So, this a is an example of the symmetric matrix, while if you look at the B, then you will say, this you know, this is not equals to this so; that means, here I have 1 2 this is a element 1 2 is not same as 2 1, but here this 1 2 is equal to 2 1, that is 1, fine?

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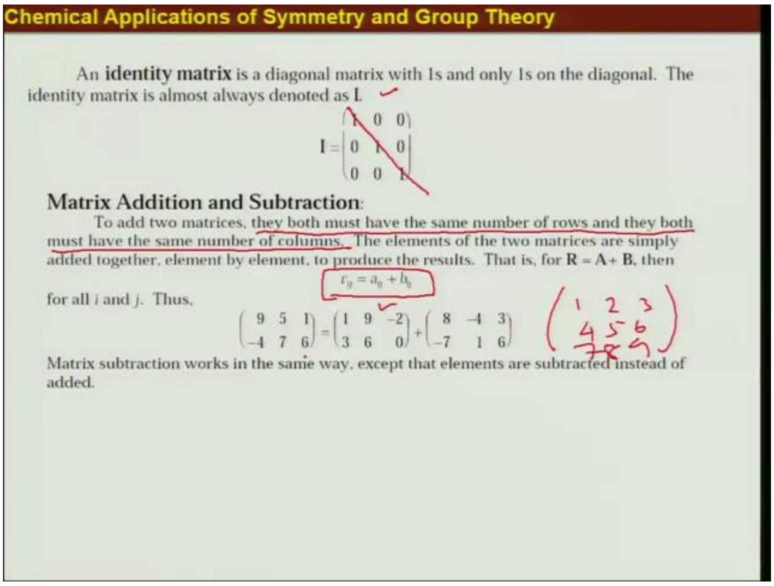

Some more definitions here, so what is an Identity Matrix? Identity matrix is that particular matrix for which, the all the diagonal elements are unity. So, you know rows and columns, so, if you go to the along the diagonal, if will be like you know element 1 1 and 2 2, 3 3 and so on. So, this, for square matrix, this is the diagonal, correct? This just like a take a square and you get a diagonal for that. So, along the diagonal if you look, at you will see that all the elements are unity and rest of the elements are 0s. So, this is called Identity Matrix and all the time Identity Matrix is denoted by this symbol I, capital I, this is a normal convention.

So, now, if you have 2 matrices and you want to do subtraction or you know, addition, with those 2 matrices, how do you do that? So, to add 2 matrices, then you know, you cannot do it with, with any 2 matrix. So, they both must have the same number of rows and they both must have the same number of columns. So, if I have say, 2 by 3 matrixes and then I have a 4 by 4 matrix, then I cannot do any kind of subtraction or addition, using these 2 matrices. The reason will be you know like this, because for any addition, the elements of 2 matrices are added together and this is done by element by element.

So, if I have matrix like here, from here. So, I have like in the first row 1 9 and minus 2 and on, on the other hand other matrix I have, 8 minus 4, 3. So, one can map 1 2 1. So, 1 plus 8, 9 plus minus 4 and minus 2 plus 3, I can have this 1 2 1 addition or 1 2 1 subtraction, but if would have matrix something like you know, 1 2 3 4 5 6 7 8 9, I could not add this to this matrix. Because the first row, second row, would be fine, but the third row it will not work. So, I cannot this element by element addition. So, that is the condition of this you know, addition and subtraction and how you do it I told you and this is specifically mentioned here and this is true for both subtraction as well as addition.

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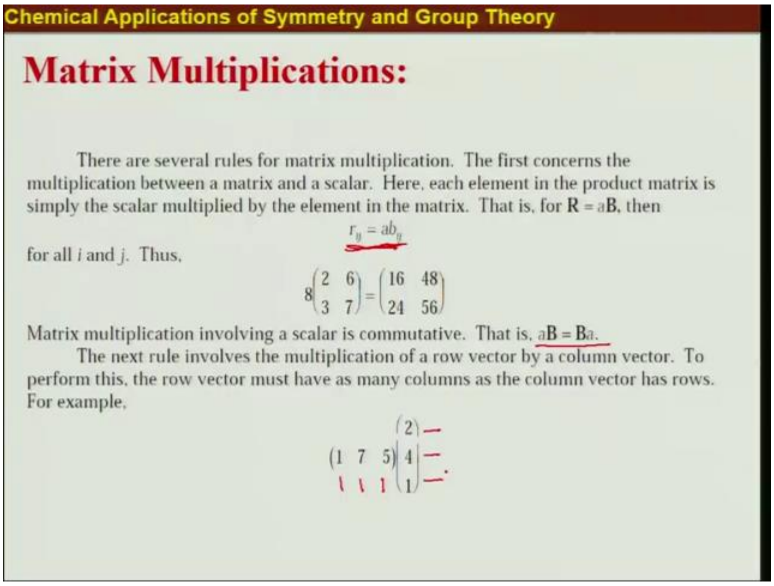

Now, whatever matrix multiplication? Because this is something which we will use very often, in case of group theory, when we use this matrices to represents symmetry operations, we need to do, you know, like 2 successive operations. So, it means like you know, operation a, followed by operation B. So, when we will try to use matrices to represent these symmetry operations, then these matrices will be multiplied and that is why this quite important in our context. So, there are certain rules for matrix multiplication, which are you know scripted here. So, the first one, it consist the multiplications between the matrix and the scalar. So, if you are given any matrix or any order and you have given the scalar and you have to multiply the scalar to this in a matrix, then it is simply multiplying each element of the matrix, by this scalar quantity, then you get a multiplication.

So, for you know any matrix b, whose element is b i j and if you have given, given as scalar quantity a, then the new matrix that we form after the multiplication, its element r i j, will be related to a and b i j and as follows. So, it is essentially multiply all the element of the matrix b, by the scalar quantity. So, one example is given here, were you can see that 8 is a square, is a scalar quantity and you have this 2 by 2 matrix. So, 8 is been multiplied with each of the element. So, 8 2 you get 16, 8 6 you get 48 and so on. So, one important aspect of this scalar multiplication with matrix is it, its commutative nature. So, it does not matter whether you multiply the, you know, matrix with this scalar or you know scalar with matrix, so order does not matter. Whatever we do the result will be the same. So, that is stated here, aB equals to Ba.

Now, the most important rule here is as follows. So, it in these rules involves the multiplication of a row vector by a column vector. Now to perform this, the row vector must have has many columns has the columns vector has. So, it says, that if you take any row vector. So, it is just a row that is called a row vector. So, you have like, 1 row and n number of columns. So, you do not have more than 1 row. So, this is called a row vector and the column vector is, just as you know 1 column and you can have n number of rows. So, only when you can have this multiplication, when this row vector has the number of columns, which is equal to the number of rows that the column vector has. So, that is shown by an example here. So, here, this is a row vector that has 3 columns, it can be multiplied with a column vector, that has 3 rows, if I would have 2 rows from the column vector or 4 rows from the column vector, I could not do this multiplication. So, this is very, very important rule and this immediately tells you, that you cannot have multiplication between, any 2 matrices that has to follow this criteria.

So, this has been shown by column vector and row vector, but this applicable to the matrix as a whole.

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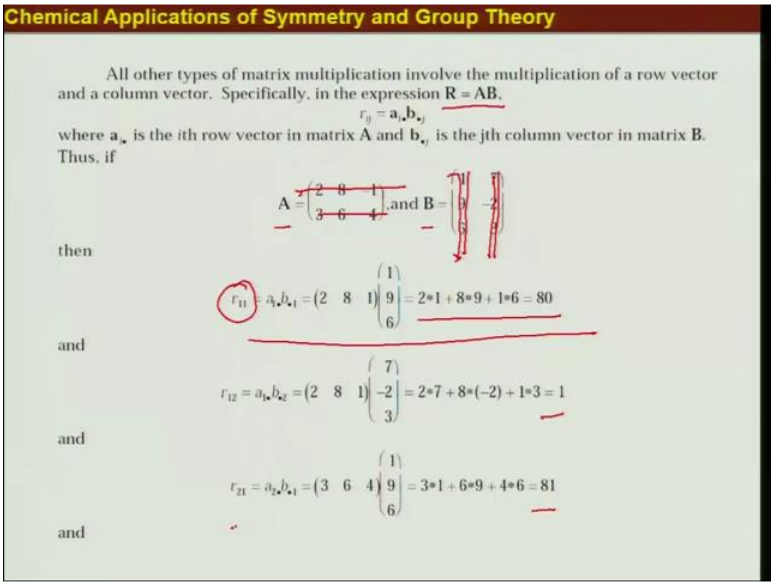

So, all the other type of matrix multiplication, involve the multiplication of a row vector and a column vector. So, you can, you can you know imagine any given matrix of whatever order, as you know, as a you know ensemble of several row vectors, several column vectors, in general, if you want to do matrix multiplication. So, it will just involve multiplication of a row vector and the column vector, like we showed just in the previous slide.

So, specifically, in the expression R equal to AB, where a and b are 2 matrices and r is the resultant matrix of the multiplication. And you know this, this small r and small b, they represents the elements of those matrices r a and b, which are been in capital and in bold form. So, here you can see that, this r i j equal to a i dot and b dot j, where this a i dot is the ith row vector, in matrix a and b dot j is the jth column vector in matrix b. Now you see that you know the number corresponding to the to the column, for a matrix is give as dot and same dot is given for the you know, the number of row, for the element corresponding to b matrix. So, these 2 dots are same, meaning that their numbers are same and then only we can do the multiplication. So, following, that you have an example here, where you have taken this a and b and a is matrix whose as 2 row 3 columns, while b is a matrix having 3 rows and 2 column. So, you can do multiplications like this. So, rule of thumb is, when you do multiplication, you know multiply one matrix to another, you do it in this way.

So, first you, you know follow this and you follow this, next again you, you know multiply with this one, then you do with using this one and then again this one. So, we follow like a row and then column and you have it like, here like you know, one element multiplied to another element and then you keep doing the multiplication and sum then all together, which is explicitly shown here. So, this is the, you know, resultant element r 11 and this how you do the multiplication. So, 1 2 1 correspond is here and ultimately you get the respective values, which will active has the element of the resultant matrix. So, you get r 11 and r 12. So, 11 as I said, it follows the first row of the first matrix and multiplies with the first column of the second matrix and r 12 will be the first row of the first matrix, multiplied to the second column of the second matrix, in that way it will keep going and ultimately you will get all the elements of the resulted matrix and ultimately you have product like this.

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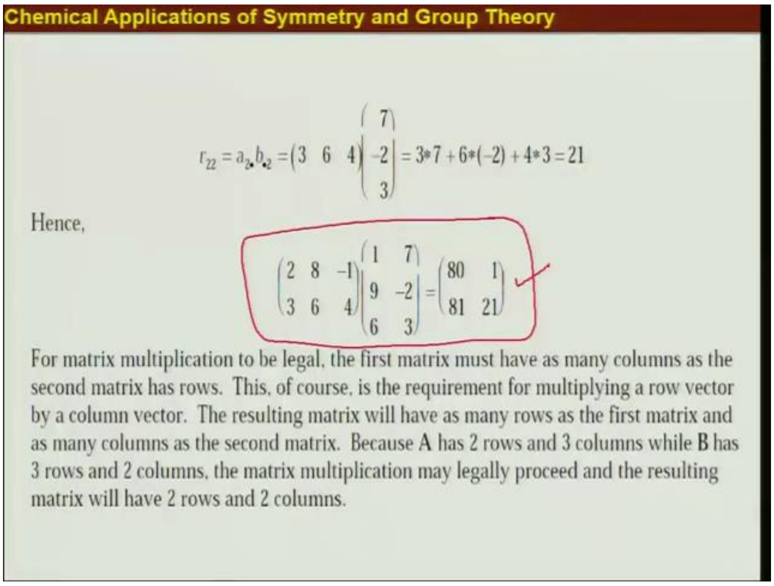

Now, this is interesting right? You had like, a matrix with 3, 2 rows and 3 columns, which multiplies with matrix having 3 rows and 2 columns and then the produce is 2 by 2 matrix, having 2 row and 2 columns. So, for matrix multiplication to be legal, the first matrix must have has many columns as the second matrix has rows, that your probably understood by now, we will get the example of the you know condition of the row vector and column vector, if you just extent that to any given form of matrix, then you come to this particular rule, which was talking about right now. So, for again, if we state the sentence, so, for the matrix multiplication to be legal, the first matrix must have has many columns as the second matrix has rows. This of course, is the requirement for multiplying a row vector by a column vector.

The resulting matrix will have has many rows, as the first matrix and as many columns as the second matrix. So, that is why you are getting this 2 by 2 matrix, because the first matrix had rows and second matrix had 2 columns. So, number of rows of the first matrix and number of column of the second matrix will give you the total dimension of the matrix that is resultant. So, that is about the matrix multiplication.

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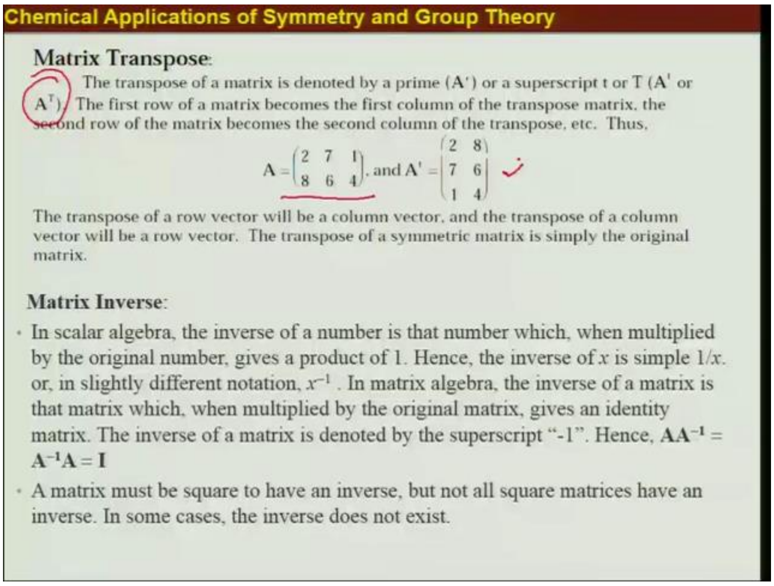

Now, there are certain other properties of matrix that we will look at now. One is the transpose of the matrix, this is the name something which is important in our particularly, particularly our context. So, the transpose matrix is a denoted by you know, a superscript T and sometime it is also written as A prime or with A superscript small t, but normally we use with A superscript t, plus T is capital letter, alright. So, that is the symbol of the transpose, now what is the transpose. So, the first row of a matrix becomes a first column of the, you know, transpose matrix. So, I had say, you know, matrix having 3 rows and 3 columns or say 3 row and 2 columns. So, this matrix, when I will transpose, it will become like, you know, matrix having 2 rows and 3 columns.

Here is one example, where a is a matrix, having 2 rows and 3 columns and that when I transpose it, it becomes 3 rows and 2 columns. So, the transpose of a row vector will be a column vector; obviously and the transpose of a column vector will be a row vector, has to be, the transpose of a symmetric matrix is simply the original matrix. So, you know in symmetric matrix what we found that, any r i j equals to r j i, if r i j and r j i are the element of the matrix. So, in that case if you know, if just make a transpose, you are not going to get something new. So, for symmetric matrix the transpose will return you the same matrix, alright.

Next we need to know, what is the inverse of the matrix. So, in scalar algebra, the inverse of a number is that number, which when multiplied by the original number, gives a product of the unity, hence the inverse of x is simply 1 upon x, because on the multiplication x into 1 upon x, will give me 1. Or in slightly different notation, I can write it x inverse. So, x inverse, we are familiar with that already. Now in Matrix Algebra the inverse of the matrix is that matrix, which when multiplied by the original matrix, gives an identity. So, the notation remains the same. So, here in case of Matrix Algebra, what you have, I have a matrix and if I need to find out the inverse matrix, then the inverse matrix will be such that if I multiply this original matrix with this inverse, I will get a matrix which is Identity Matrix. So, the inverse of a matrix is denoted by the superscript inverse, so, it is a inverse sine. So, if I write same matrix by capital l, A, in bold letter. So, inverse of the matrix will be capital A in bold letter, inverse.

So, it is implied that, the you know, AA inverse is equal to A inverse A, that is they commute and the result is identity. And the in order to have an inverse, in other words, for the inverse of a matrix to exist, the matrix must be a square matrix; that means, the number of rows and numbers of columns must be equal, but the reverse is not always true. So, all the square matrices may not have inverse, in some case, inverse does not exist.

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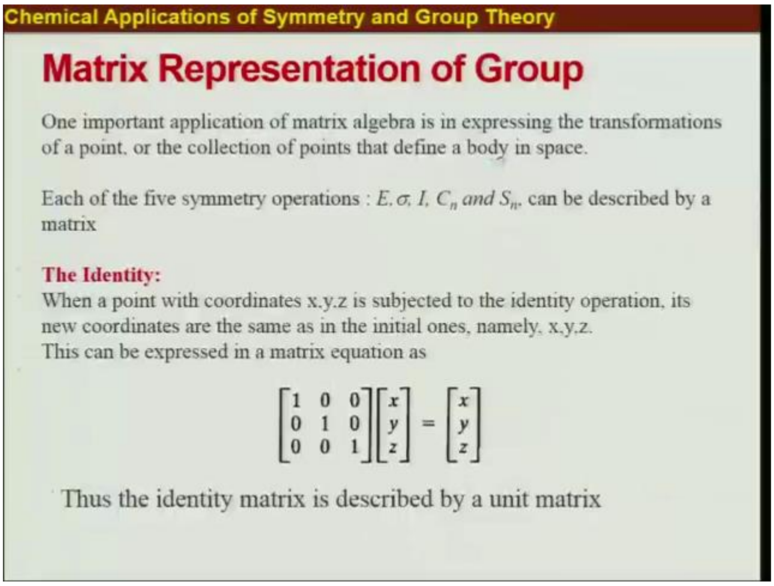

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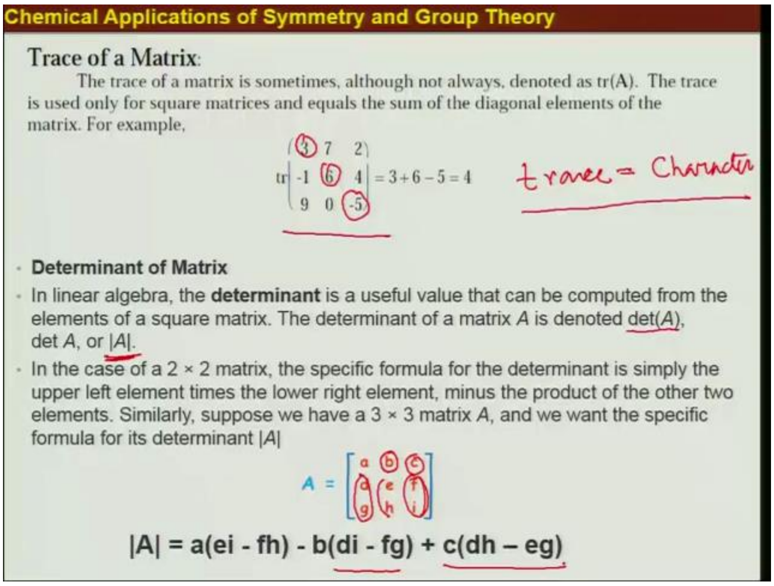

Before we go to the representation of group using matrix, we learn couple of more things; one is the trace of the matrix. This is something which you will be using throughout the course, hence forth, once we go through the representation. So, trace of a matrix is the sum of the diagonal elements of the matrix, if I look at any given matrix, say on the matrix on the screen, here, the sum of 3, 6 and minus 5, will give the trace of the matrix.

So, this has you know very important consequence, particularly under context of you know, symmetric point groups and then representation and you will soon learn that, this trace of matrix, particularly certain matrix which can be in a block factor, to a form by you have only the diagonal elements and the off diagonal elements are 0, in this cases this trace of those matrices, will be some what characteristics of this particular matrices, that in term represent certain symmetry you know, operation or you know in case of group we are talking about, then it will represent the you know any particular group element. So, this trace, in the context of group theory, we will be using the term, character. But till now, we will just you know stick to this terminology, phase, until unless we go to the representation of the group and we will also learn then why these trace is called the character, but for your information, you should know the this trace, will be actually acting as character of any representation, very well.

And the one more thing I would like to mention here is about the determinant of a matrix. So, how many of already know what determinant is. So, the determinant is a useful value that can be computed from the elements of a square matrix. So, the determinant of a matrix a. is denoted as either this term or this symbol. In the case of a 2 by 2 matrix, the specific formula for the determinant is simply the upper left elements times, the lower right element, minus the product of the other 2 elements. So, if you have a 3 by 3 matrix, then we can determine the value of this whole determinant, in this fraction. So, you have, this a fix and then you find out about the this particular part and then you subtract, you know, a part where you know b is multiplied with the determinant, which is consist of this 2 terms, on your screen here you can see and then you do it for the c term. So, in this way you can find out about the determinant of any order. So, if you have a square matrix of any given order, we can find the value for that, you know, determinant.

So, with that we will stop here today and in the next class we will come back, with same representation of the symmetry operations, where you will use this you know this brief knowledge of Matrix Algebra, that is we learnt today and we will use them and try to find out about, you know, representation of the symmetry operations.

Thank you for your attention, see you tomorrow.