Symmetry and Group Theory Prof. Dr. Jeetender Chugh Department of Chemistry and Biology Indian Institute of Science Education Research, Pune

Lecture - 03 Symmetry Elements and Operations - Part 1

Welcome back everyone. So, welcome to lecture 2. So, in last class we have seen that how symmetry actually plays an important role in mathematical functions in helping us solve some of the integrals. Like we took one example where we can see how symmetry in mathematical functions could actually help us solve integrals, but that is only one part. Let us now go back to symmetry in real life, symmetry in molecules. And see what are symmetry elements? What are symmetry operations and how we can classify molecules based on symmetry?

(Refer Slide Time: 00:56)

Lecture 2 Symmetry: of Symmetry dements = Geometrical entities, point, line as a plane about which a symm of a be consident Symmetry operation = Movement of an object about a set of points which hermain warnared resulting hits a convicted configuration of the abject. points which remain unmared resulting

So, let us start with lecture 2. And we will be looking at in more details. What is symmetry about? So, we are all aware of symmetry, right. As we discussed in the introduction lecture that we see flowers around us. There is some sense of symmetry, when we see flowers, right. Then, let us say we are hanging a photo frame on a wall. So, we always wanted to be perfectly horizontal. So, we have some sense of symmetry that it looks beautiful when there is symmetry around.

So, we already are aware of concept of symmetry, it is just that we have to identify the concept of symmetry with respect to molecules around us, in small molecules, big molecules and so on. So, in this course, particularly, we will be looking at symmetry molecules, and then we will try to understand what are symmetry elements? What are symmetry operations? So, we will be defining these terms today?

And then on the basis of symmetry elements, and symmetry operations, can we classified molecules and group them and then correlate it with physical properties? So that part will come later. So, let us look at symmetry elements and symmetry operations. So, symmetry elements and then we will go to group definition later. So, symmetry elements are geometrical entities like point, line, or a plane about which a symmetry operation can be carried out. So, you can see by defining symmetry elements, we also have to invoke the term symmetry operation.

So, you cannot define symmetry element without symmetry operation, so, when you are defining symmetry elements symmetry operation term comes and similarly, when you are defining symmetry operation, symmetry element will come. So, let us say if we are defining now, symmetry operation. So, symmetry operation is movement of an object, in this case, molecules or a molecule, so, movement of an object about a set of points, which remain unmoved resulting into an equivalent configuration of the object. We will take example, so do not worry if it is not clear, but let us just first get done with the formal definitions. So, what is a symmetry operation, symmetry operation is movement of an object about a set of points. Now, these set of points what are these set of points, a set of points we will see which remain unmoved.

So, since these are remaining unmoved by movement of an object, these are called as symmetry elements. So, basically symmetry operation is movement of an object about symmetry element resulting into an equivalent configuration of the object. So, again, so symmetry operation when you are defining, so symmetry element is coming in the definition. So, both of the terms are related and you cannot define one without the other. So, we will always be talking symmetry elements and symmetry operations together.

(Refer Slide Time: 06:03)

Effect of a symm operation: To take the object into an tech symme of must have a symme element There are 5 different types of Symm elements and Required to specify

So, let us look at some more examples. So, let see, what is the effect of a symmetry operation what is the effect? So, you can probably think about it now, to take the object into an equivalent configuration. And each symmetry operation must have a symmetry element. So, I am emphasizing this, because it is very important that this difference between symmetry element and symmetry operation is very very clear in our heads, because it is really important further down the line.

So, we should be very well aware of what is a symmetry element, symmetry element is a geometrical entity, like point, line, or a plane about which a symmetry operation is carried out. And symmetry operation is the actual movement of an object. So, let us not get confused between symmetry element and symmetry operation. So, let us say if we are carrying a rotation, so let us say this is an equilateral triangle. Let us define the vertices as 1, 2, 3.

Now, let us say you are rotating this let us say that there is an axis which is passing through the center of this and this axis is perpendicular to the plane of the board. So, axis perpendicular to the plane of this board. Now, you do a rotation about this axis and rotate it by let us say 120 degrees. And all the rotations in this class will be anticlockwise. So, you rotate it by anticlockwise 120 degree, what you get this 1 goes to this position 3 goes to 2.

So, you have 3 here and 2 here. So, now, the triangle looks exactly the same, the triangle is now called, as that it has reached in an equivalent configuration, because of this moment, so now this

movement is called as a symmetry operation, whereas this axis is called as symmetry element. So, the triangle is called is to have that, there is a symmetry element present, about which a symmetry operation can be carried out, so that it reaches to equivalent configuration.

So, this should be very very clear now in our heads that what is a symmetry element and what is a symmetry operation? So now let us say let us try to define all the symmetry elements and operations which are required to specify molecular symmetry. So, there are 5 different types of symmetry elements and corresponding operations which are required to specify molecular symmetry. So, let us look at this one by one.

(Refer Slide Time: 11:13)

Symm Element Symm Operation Symbol 1) Identity No movement E 2) Plane of Symm Reflection through T the plane Tr., To, Th 3) Center of Symm Inversion of all peints i (Inversion Center) (an atom) thru the center 4) Proper axis of potation

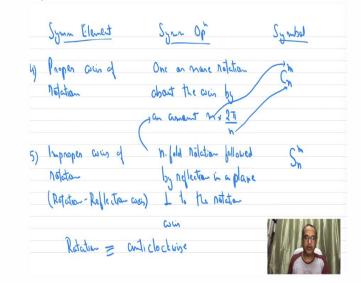
Let us go to let us make a table of a symmetry element, then corresponding symmetry operation, and what is the symbol that is used for the corresponding symmetry operation or the element. So, the first one is called us identity. So, symmetry element will again discuss this in more details let us let me first list it down. So, first symmetry element is called us identity, the corresponding symmetry operation is no movement.

So, you do not move the molecule in this case. So, if you do not move the molecule will always be in equivalent position to itself. So, we call this and the symbol corresponding to this is E, capital E, uppercase E. So, identity operation and identity symmetry element. Now, let us look at the second one. Second is plane of symmetry. The corresponding symmetry operation Yes, you have guessed it right, it is a reflection through the plane, and the symbol is sigma. And there are 3 types of planes. One is sigma v, sigma d, and sigma h. We will see in details, this is called as vertical plane of symmetry, dihedral plane of symmetry, and horizontal plane of symmetry. Third is center of symmetry. In some books, you will also see it as center of inversion or inversion center, they all mean the same thing. The corresponding operation is inversion of all points (or you can say atoms because we are dealing with molecules) through the center.

So, we will be inverting we will see again how to do this how to perform the symmetry operation. This is just the definition - Inversion of all points or atoms through this center and it is denoted as lowercase letter i.

The 4th is proper axis of rotation. Let me go to next page.





So we had symmetry element, symmetry operation, and the corresponding symbol, right, and we were looking at proper axis of rotation. Now, the corresponding operation is one or more rotations about the axis and also say by an amount m x 2pi / n. So, let us see what is m what is n more in details and the typical symbols are Cn to the power m. So, n is this n 2pi / n and this m goes over here this n was here.

So, if something is there is a proper axis of rotation then there also has to be an improper axis of rotation. It is also called as rotation-reflection axis now, the corresponding symmetry operation is

n-fold rotation, this rotation is actually same as this one for proper axis of rotation, but this is coupled with or followed by (there are 2 operations in one improper axis of rotation) first operation is n-fold rotation followed by reflection in a plane, which is perpendicular to the rotation axis. We will see again by examples it will be clear, but let us see.

So, in the same nomenclature as Cn [^]m this is described as Sn [^]m. So, m times 2pi / n followed by a reflection in a plane perpendicular to this rotation and again whenever I am doing any rotation, so, all the rotation in this class will be anticlockwise. So, it really does not matter, but you have to follow one convention throughout so that you are you do not make mistakes. So, if you are following clockwise rotations, you can follow clockwise rotation there is no harm in that you will get the same answers. Your intermediary steps may have different configurations but the ultimate answer to any given problem would be same.

But for the sake of convenience you can keep following any particular one. So, if you are following clockwise, keep following clockwise I like to follow anticlockwise So, I will be following anticlockwise rotations.

(Refer Slide Time: 19:30)

E (Identity) : The identity operation does nothing to the molecule. (emerpandy your element is the whele malecule. Every melecule has afleast the dement. Importance: Same as the importance of digit 1. I is neguined to define inverse of a number Proper vis and proper notation ((") Rotate a malecule by <u>277</u> (<u>310</u>) and if the Notation brings the malecule into an equivalent Configuration (paritor, then Cn exist.

So, now let us look at each of the symmetry element and symmetry operations one by one, so let us start with E identity. So, as you know the identity, we have said that corresponding operation is there is no movement of the molecule. So, the identity operation does nothing to the molecule. We will say why it is required then, if you do not actually do anything, then why do we have it we will see the importance.

So, the corresponding symmetry element, so, what will be the corresponding symmetry element remember like, when we first said the symmetry element is a set of points that remain unmoved while doing the rotation or while doing while performing a symmetry operation. So, in this case the symmetry element is the whole molecule. The whole molecule itself is a symmetry element because the whole molecule itself is not moving, all the points in the molecule are remaining at its one original position.

So, then we can say that every molecule has at least this element. So, this element is ubiquitous in nature, it is present in all molecules. Every molecule has the symmetry element. Now, what is the importance of this. Why do we have it? So, importance is same as the importance of digit 1. So, for example, like 1 is required to define inverse of a number, right. So, similarly, E is required to define inverse of a symmetry operation.

So, just like 1 is required in algebra to define any inverse, E is required to define inverse of a symmetry operation. So, that is why we have E. Now let us look at the second one. So, before we actually go for symmetry, point of symmetry, or the inversion center, or the plane let us first define proper axis of rotation. So, proper axis and proper rotation, which is defined by Cn ^m. Now if you rotate, we have seen an example of rotation by rotating manipulating triangle but let us look at the actual molecules, rotate the molecule by 2pi / n or you can say 360 degrees by n, and if the rotation brings the molecule into an equivalent configuration, or some books will say position, then we can say Cn exists.

(Refer Slide Time: 25:25)

And the Symme dement is called as coins of Symme Para 27 Netalian, There is a m-fold over of Symm C, was =) Rotation in 180 (, wijo ~ 120 2

And the symmetry element is called as axis of symmetry in short or you can say proper axis of symmetry. So, for example, for a 2pi / n rotation, there is an n-fold axis of symmetry. So, if the rotation is, let us say if we say that there is a C2 axis this would imply that the rotation is yes, you guessed it right, 180 degrees, 2pi / n. So, 2pi power 2 is 180 degree. If there is a C3 axis present, the rotation is 120 degrees. So, let us now take an example, let us say draw a right-handed coordinate system x, y, z. now let me draw water molecules.

So, while drawing water molecule, I will place oxygen at origin and then the 2 protons or 2 hydrogens in yz plane. So, the angle is the standard water angle. And this is the y-z plane is the plane of the board x is coming out of the plane. This is how I am going to draw all my coordinates all the time. Now if I am carrying out, and then let us label or let me color 1 H differently so that we can differentiate the 2 hydrogens.

So now let us say if I now do a C2, which is a along z-axis. So, I am taking this axis over here, this axis, and the rotation is like this anticlockwise. And if because it is C2, so the rotation will be of 180 degrees. So now how the molecule would look like, so let us draw the molecule. So, O will remain at its own position. Now, what happens to the 2 hydrogens? The blue hydrogen will come at this point. And the red hydrogen will come at this point. But the whole molecule as such is equivalent to this molecule? So, we can say that C2 z exists.

Now let us take another example. Let us say if we do x, y, z rotation, C2 z rotation on the coordinate system itself. So let us move the whole coordinate system with respect to C2 z axis. What do you get? Minus x. Now, x goes to, if I am doing this flipping, the x will move towards minus x. So, x goes to minus x, the y will go to minus y. So, if you see this, the y will go to minus y. x will go to minus x, z remains where it was. So, x becomes minus x, y becomes minus y, z remains as z, so z did not change. So, because it is C2 z .

So, z axis remains it is at its own position because z axis is collinear with C2 axis. So, the C2 axis as we defined, because it is a symmetry element, C2 axis will not change its position. Anything which is lying about on C2 axis, for example, the oxygen was lying on the C2 axis so, oxygen itself could not change. Similarly, here z axis will not change here. So, x will go to minus x, y will go to minus y, and z will remain here. So, let us stop here and we will see more examples of proper axis of rotation in next class. So that it is very clear in our heads that how a symmetry axis or how a proper axis of rotation actually works. Thank you.