Chemical Applications of Symmetry and Group Theory
Prof. Manabendra Chandra
Department of Chemistry
Indian Institute of Technology, Kanpur

Lecture – 01

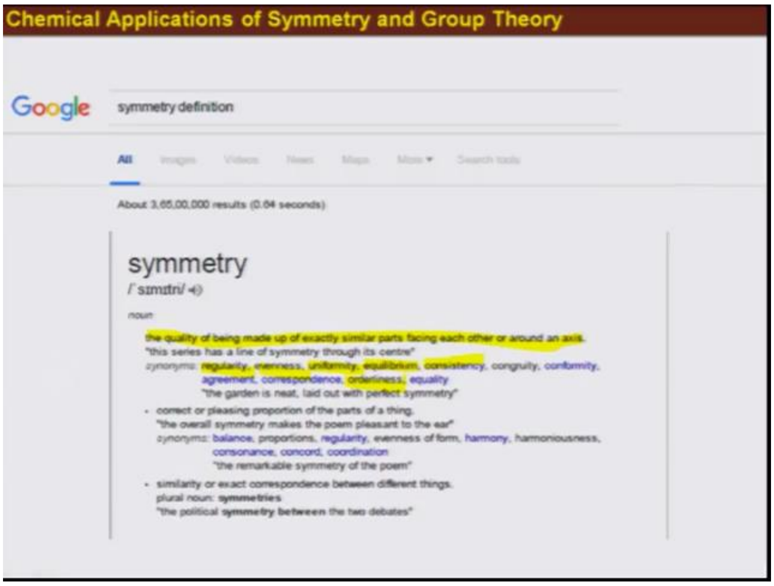
Hello and welcome to the course, whose title is Application of Symmetry and Group Theory, in chemistry. This is the first day of this lecture and I welcome you all to this course. Let us start with the introduction of this topic as a whole. So, this particular topic Symmetry and Group Theory this is of utmost importance for chemist particularly, any form of chemistry, like inorganic chemistry organic chemistry, physical chemistry and also to the audience belonging to chemical engineering, and even physicist. In chemistry particularly, say an inorganic chemist, who all you know all the time talks about, say bonding, incase of transition metal complexes.

So, in transition metal complexes say, people talks about formation of you know linear combination of atomic orbital's to form, so called, Symmetry Adapted Linear Combination. So, many of you are probably familiar with this term senior, Symmetry Adapted Linear Combinations or in short SALC. Now how this you know linear combination is formed there are certain rules, which are based on symmetry. So, that is why it is called Symmetry Adapted Linear Combination. So, one need to know what is the relation between this symmetry, of any given molecule, and the formation of this, molecular orbitals.

Similarly, spectroscopic or physical chemist, who wants to know about the possibility of a transition, from one given energy state of the molecule to another electronic state, there, knowing the symmetry of the states, or in particular, the symmetry of the wave functions, related to those electronic energy levels, or vibrational energy levels, is very much needed. So, in various aspects, we will need this molecular symmetry, the symmetry, when you say molecular symmetry what I mean is, the symmetry of the molecular structure in general, and in particular symmetry of the you know, wave functions of molecular electronics states, or vibrational states, and so on.

Now, when we talk about symmetry what comes to our mind first. So, let us have a look at the result that we obtained, by putting the term Symmetry in a Google page. So, here it is.

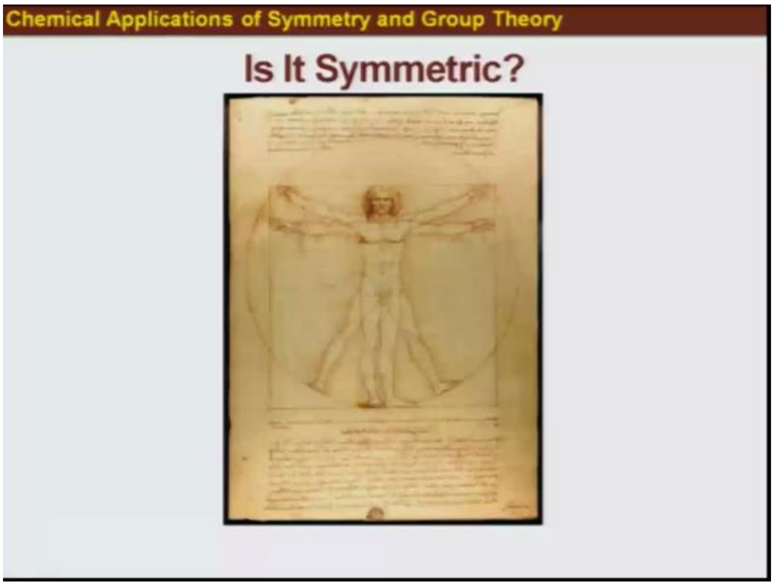
(Refer Slide Time: 03:15)



You can see there you know a definition of Symmetry is given here, which says like the quality of being made up of exactly similar parts, facing each other or around an axis, which also tells you, that you know if I can highlight that portion. So, this is the definition that is given by a search in Google, and there are so many synonyms that are provided like regularity, uniformity, evenness, or equilibrium, consistency, orderliness. So, all these things give us some picture, about symmetry, symmetry of an object, symmetry of a molecule, molecular structure and all. So, suppose you know give I you a molecular structure, or any object at a place you like I give you this one, the mouse, and I ask you what do you think about its symmetry? What will be an answer? Probably you will tell well it is to some extent, symmetry.

So, let us have a look at certain objects, and try to see if we can say something about their symmetric. At least are they symmetric to us? Or do the same to be symmetric? Or we do not find any symmetry in those structures? Or you know, we can say like this is more symmetric then other ok.

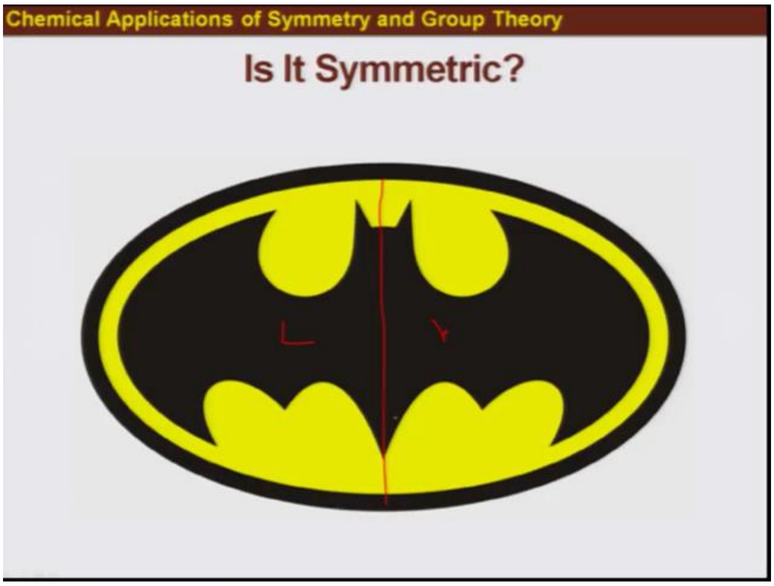
(Refer Slide Time: 04:54)



So, here is famous picture, many of you will probably know, this is a drawing by the great Leonardo Da Vinci. This is virtuous man. So, this is the description of a human body, at two different orientations.

Now, looking at this, what you can you know, say about the symmetry of this human body? The obvious answer will be well, this is very much symmetry. We have been reading about it in even in our biology courses, the human body, or you know animal bodies, there symmetric, ok. So, let us have a look at some of the other structure that we can think of.

(Refer Slide Time: 05:39)

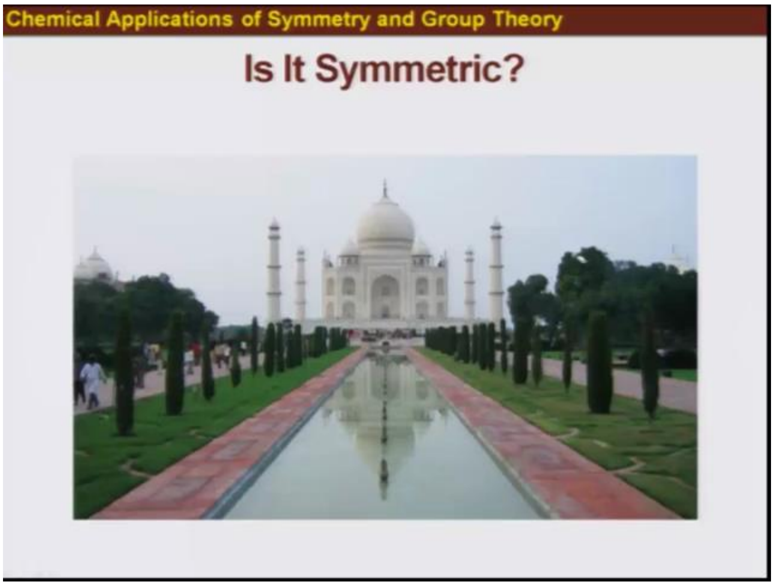


You obviously know this one, is famous symbol of you know in the batman movies right? This is picture of a bat, seemingly. So, looking at this you can say, there is some sought of symmetry, you can say that, why? because if you if you look at the object, in this fashion where you look at you know this part, the right side part and the left side part of this object, about this line, then you can say that those two halves are almost like a mirror image, not almost like its a mirror image of each other. So, we can say this is symmetry, a symmetric object.

(Refer Slide Time: 06:30)

So, similarly if I look at another picture; let me erase those things. So, here also, this is the picture of bird, a beautiful bird here, and you can see that about the, you know the mid portion of this birds body, you can see is pretty must like a mirror image, both the sides the wings and the tail, you can just dissect it in the two equal halves. So, to you it will be like very symmetric, object.

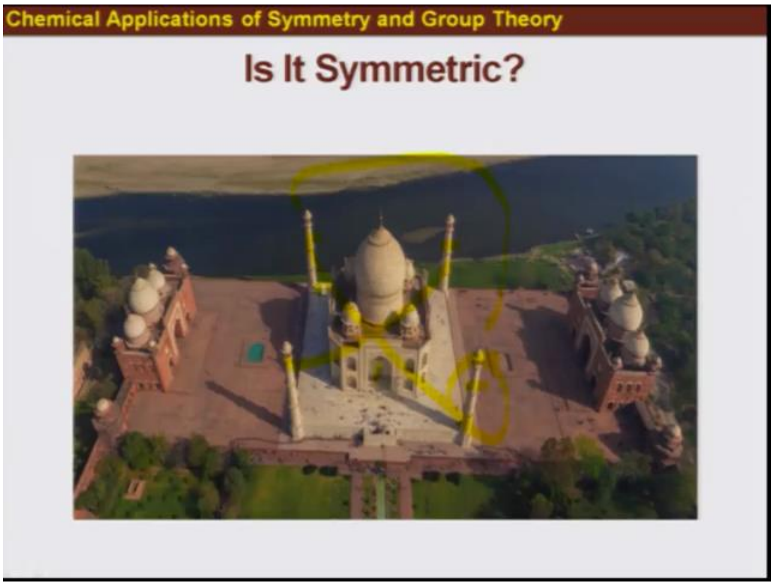
(Refer Slide Time: 07:05)



Now here comes, one of the, you know, Seven Wonders of the World is the great Taj Mahal.

So, looking at this phenomenal architecture, you can at first say is very, very symmetric, and you know observation is very true.

(Refer Slide Time: 07:20)



Particularly when you look at from a top view, that is an aerial view of Taj Mahal, you can see how nicely this you know architecture was built. So, look at, there are four domes, one here, one here, one here, one here, the doors here. So, you will find the same pattern of doors on each side, on each side of this Taj Mahal. So, if you start from say one dome, and go through the center part, you will reach the other dome. Similarly here if you come through this center of the Taj Mahal, you can reach the other dome, fine? And if you a standing suppose near this dome, and look at Taj Mahal, and then you go all the way to here, and stand here, and look at the Taj Mahal, you will not find any difference between your views. So, that is why, this is symmetry, and when I say go back and say like I showed you the, you know, picture of the bird, and now I am show you this picture of Taj Mahal. You will probably say well to me, Taj Mahal seems to be more symmetric than the bird. So, let us look at some of the other structures, that we can you know, that we see almost every other time.

(Refer Slide Time: 08:44)

This is a famous lotus example, lotus temple sorry; this is also a very, very symmetric. So, you can you can easily see that is very symmetric structure.

(Refer Slide Time: 09:15)

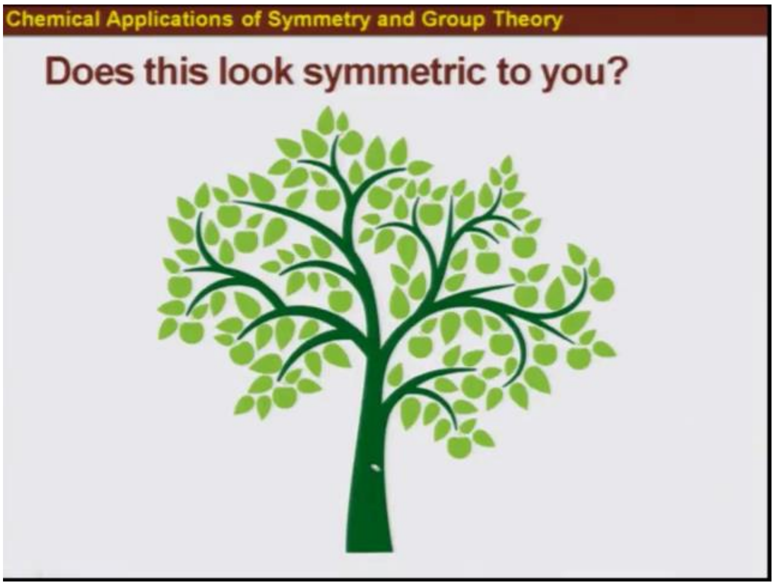
Now, let us look at some of the other structures here it also looks pretty symmetry.

(Refer Slide Time: 09:20)

Here it is the, a, building, famous building, many of you know, this is called Pentagon, the probably the head office of US Defense. Now this is also highly symmetric. Now when you say this, that this is very symmetric and one is probably more symmetric than others, then how do we say that, how can we say one structure is more symmetric then other structure, we will know how to do that. Now we have seen some structures which we can say that, all of them are to some extent symmetric, some are you know more symmetric, some are less symmetric, but overall symmetry.

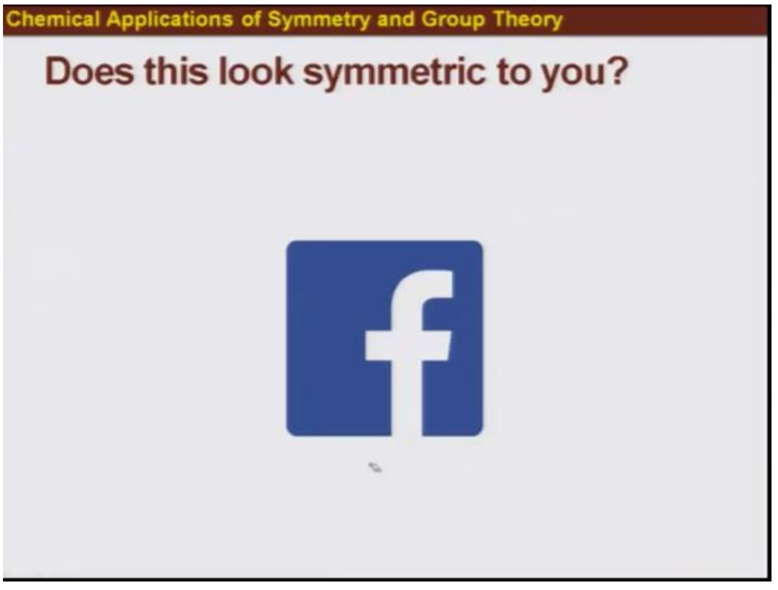
Now, let us have a look at this and how does it look.

(Refer Slide Time: 10:05).



Does it look symmetric to you? This is the picture of tree which has like an arbitrary shape. So, if I ask you, where it is symmetric or not - you will say there is no symmetry. So, you can feel intuitively, whether a structure is symmetric or not. So, so far, all of us you know, we have developed some sort of intuition so that we can say it is symmetric or not. Let us have a look at some of the other structures Facebook symbol.

(Refer Slide Time: 10:39)

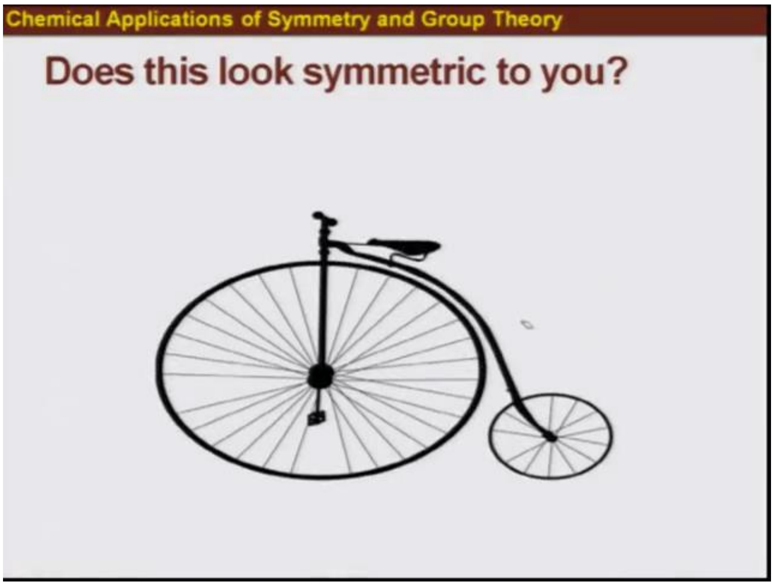


If I ask you will say it is not symmetric, because you know when we looked at the symmetric structures, we could start from one particular point, and go to another direction, and ultimately we will you know find almost equivalent point and the other side. Here we do not have something like that. So, no two points in this particular Facebook has the same environment, this face book you know logo. So, we can call this, and this is not symmetric.

(Refer Slide Time: 11:16)

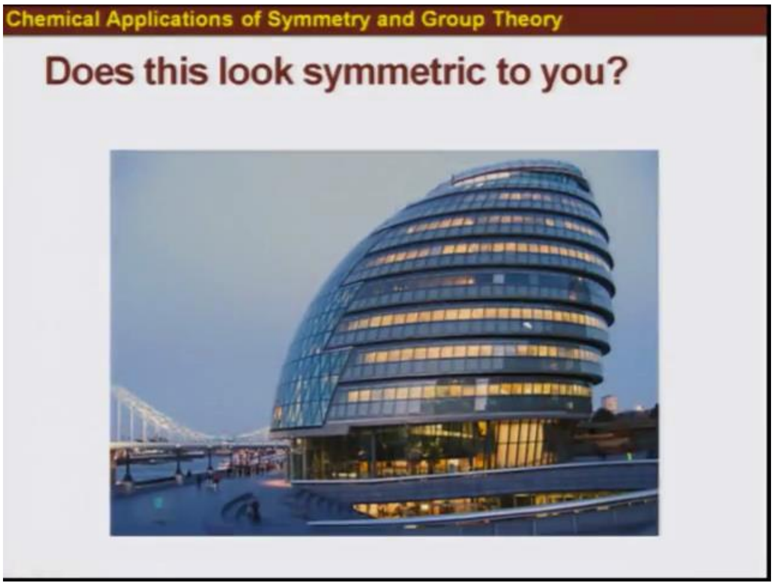
Now, same is here is a zig zag railway track, I do not find any symmetric here.

(Refer Slide Time: 11:22)



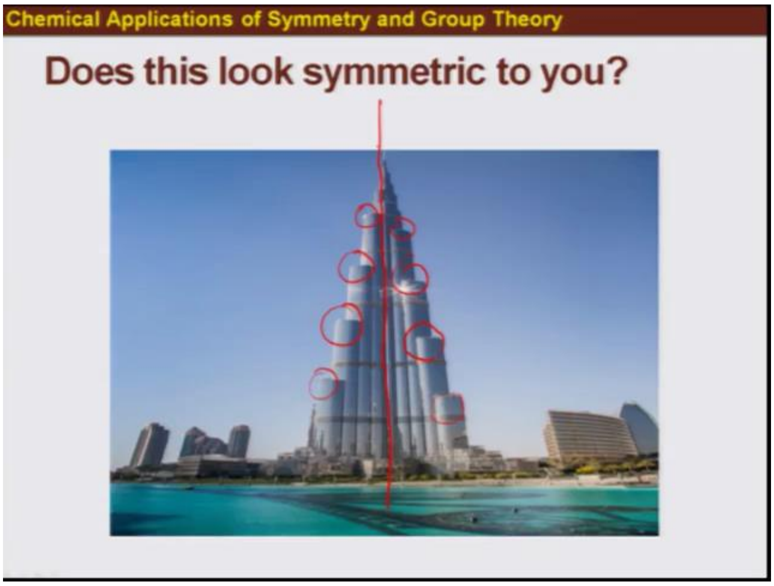
The oldest bicycle with the bell, I do not see any symmetric.

(Refer Slide Time: 11:25)



Here is a building, amazing, but does not look symmetric.

(Refer Slide Time: 11:31)



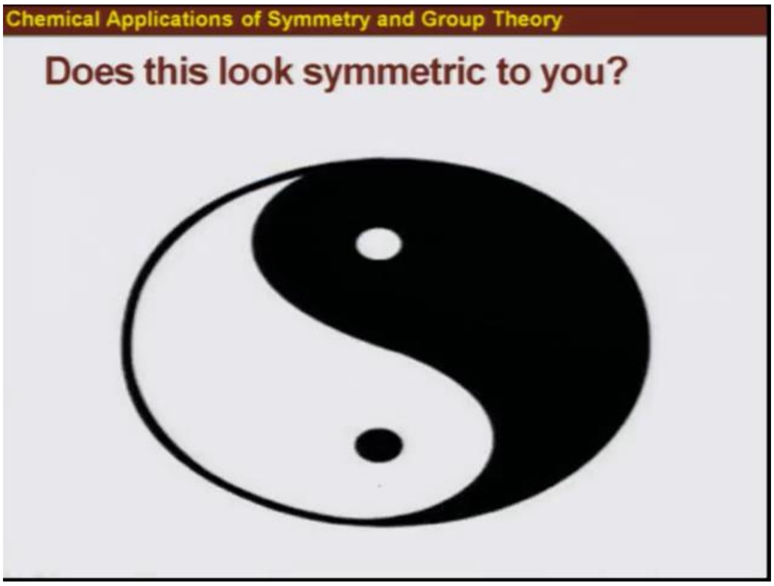
A famous classic example of, you know, building which is known as Burj Khalifa, many of you have probably seen the picture of this.

Now, apparently it looks symmetric, but a close look at this building will you know, tell you that this is not symmetry, which will be obvious, if I tell you. See if I can mark these places. So, there is a central line through this one, and then, if it is symmetric, then both the side should be equivalent right? So, if I look at you know, a part of the building, here and here, they are not same, their heights are different, same things here and here, here and here, here and here all through. So, this is not actually symmetry, though apparently it looks like symmetry.

(Refer Slide Time: 12:30)

So, the, the thing that I want to you know, convey to you, that by looking at the structures, we can say whether they are symmetric or not.

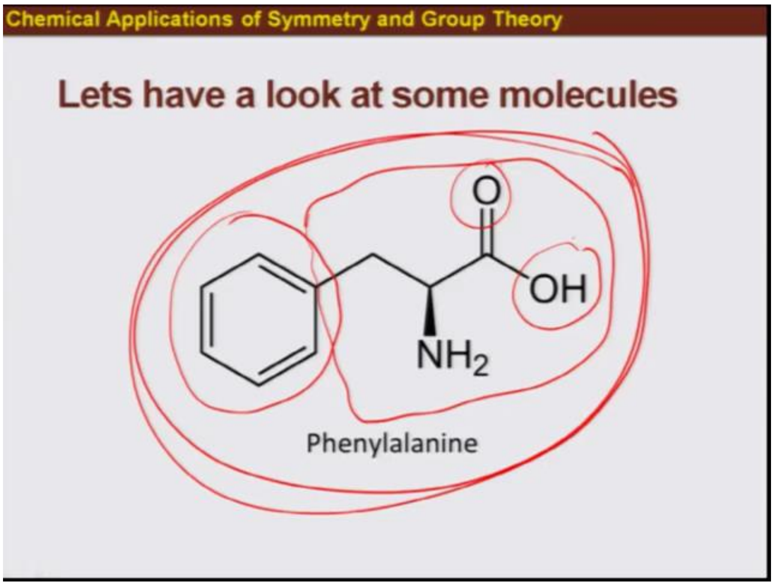
(Refer Slide Time: 12:32).



So, now, we have been, so far, we have been talking about the symmetry of objects, like buildings or creatures, architect, architectures, now ultimately we are going to deal with the symmetry of molecular systems right? So, let us have a look at certain molecular structure, and then let see if we can comment about their symmetries.

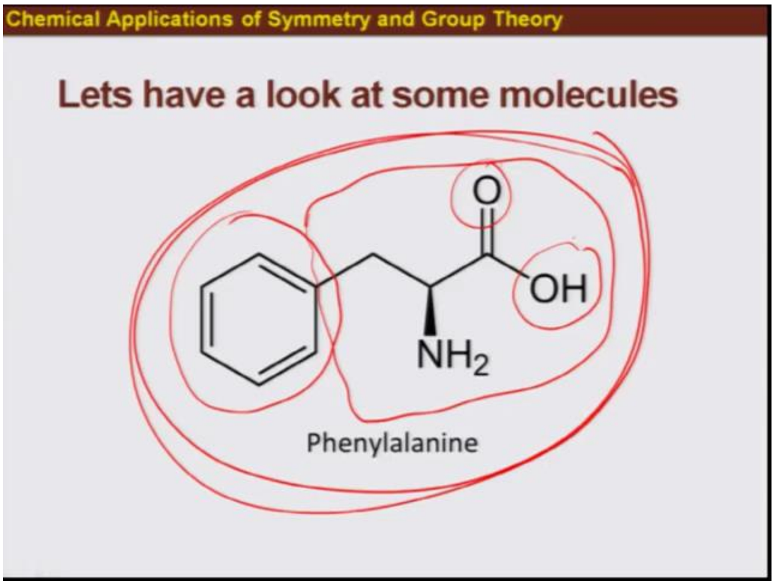
So, let us have a look a molecule called phenylalanine.

(Refer Slide Time: 13:12)



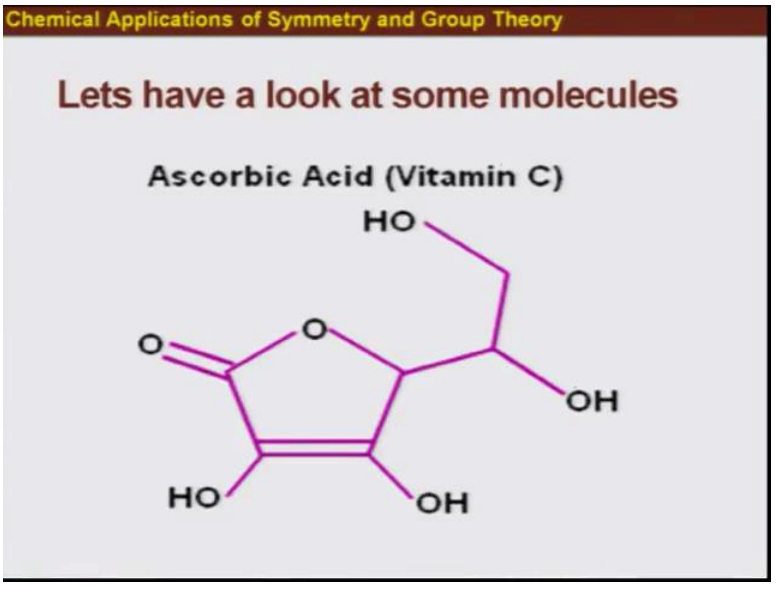
So, this is phenylalanine is a minus (Refer Time: 13:23) Now for a second, you forget this part. So, this benzene, wait just only the benzene, if you look at its, its very much you know symmetric to you right? So, any you know, point on this object can find an equivalent point on the other side of the molecule, but as a whole, when I talk about this phenylalanine I have you know molecular structure, where you have this ameen group projecting outside, the plane of the molecule, and this c double point o, or o h, they are in the plane of the molecule. So, overall it does not seem to be and symmetric molecule, which is obvious.

(Refer Slide Time: 14:08)



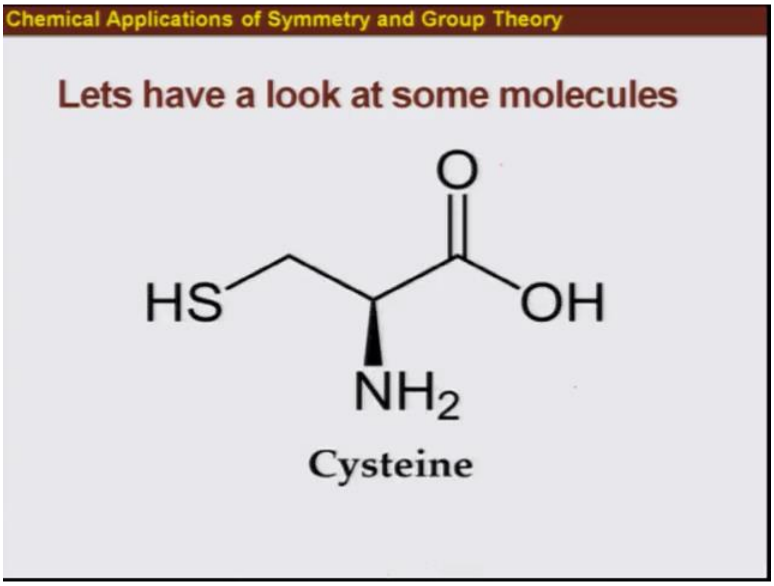
Now, similar is here for a molecule tryptophan. I do not see any symmetry in this molecular structure.

(Refer Slide Time: 14:19)



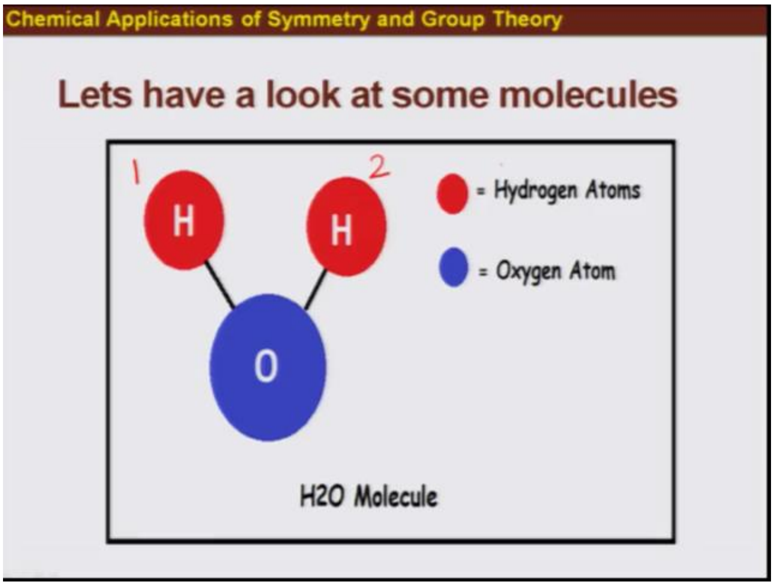
Ascorbic acid tells me the same thing, about its structure.

(Refer Slide Time: 14:24)



Cysteine, another amino acid, all is not having something which can tell me that to molecule symmetry.

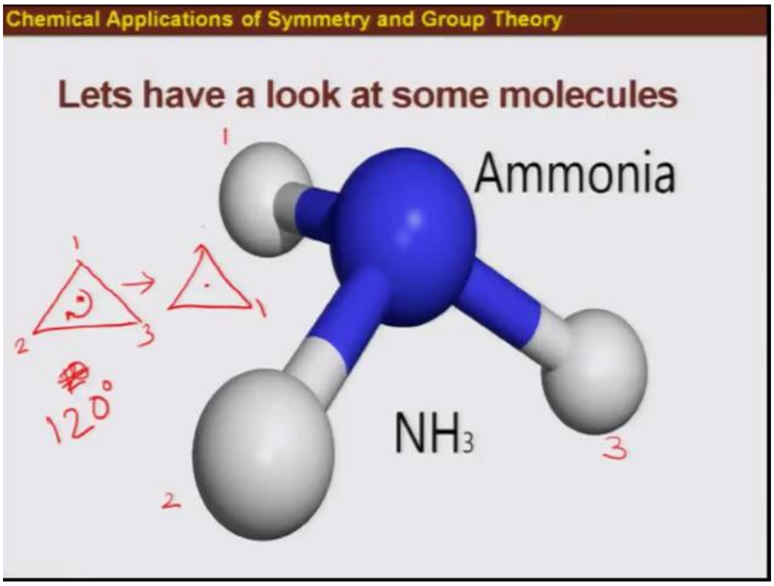
(Refer Slide Time: 14:36)



Now, let us have a look at these molecules, the most common molecule on earth, so, water. This is the structure of water, oxygen and two hydrogens a bonded. Now suppose I can somehow mark. So, before, that if I look at this molecule it seems to be somewhat symmetric to me, how? Let us try to explain that, suppose I can mark this hydrogen atom, somehow. So, I mark this hydrogen as one, and this hydrogen as two, and then. So, this water molecule is like this correct? So, one hydrogen here, another hydrogen here, and to oxygen is sitting here. Now if I interchange this one and two by some way.

Say for example, I do it like this, if this hydrogens are not marked one and two, I have no way to figure out whether there is anything, you know, any change that has happened to this molecule. So, in other way I can say that if I simply take this water molecule and then rotate by 180 degree, and if the hydrogens are not marked by numbers one and two, then I have no way to figure out that there is any difference. So, they are essentially indistinguishable. So, this is the termed that will be using many times that after doing this 180 degree rotation, I get an indistinguishable molecular structure. So, this molecule is symmetric definitely, because I can interchange two hydrogens and get an indistinguishable just structure. So, we are slightly heading toward some sort of quantification, we will come to that.

(Refer Slide Time: 16:39)

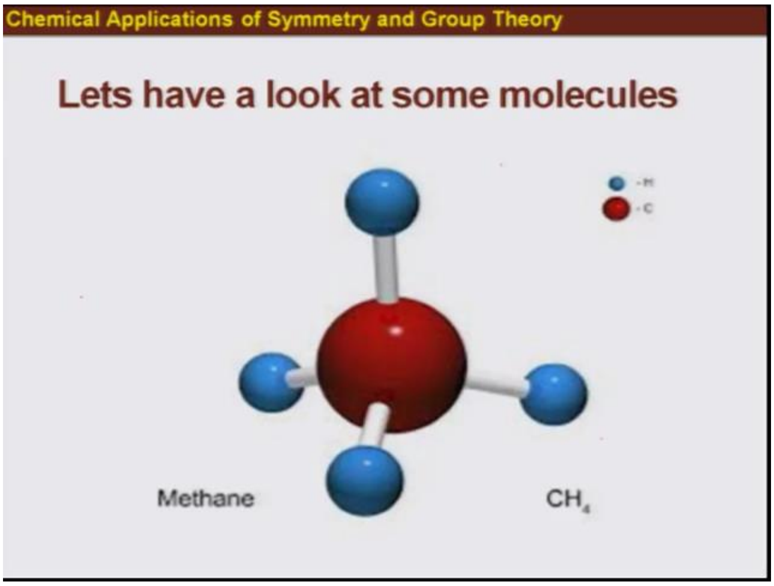


Let us have a look at another molecule, which is also very much known to us, particularly the students who have been working in, in chemistry laboratory, a organic or inorganic even physical laboratory, we know about ammonia. So, ammonia has a pyramidal structure, as you can see here. So, one nitrogen and then three hydrogens are like occupying three vertices of a triangle, like if I can draw right here. So, if I mark this place, this hydrogen atom as one, this hydrogen atom is two, and this hydrogen atom as three and add 1 2 and 3 by straight lines, I will have find something like this, and equilateral triangle, where this nitrogen is sitting from where the center, above the plane fine?

So, now I have mark this hydrogens are one two and three. So, let us mark them 1 2 and 3. Now suppose I give a rotation, about an axis which passes through the nitrogen atom, and say I give a rotation of 60 degree sorry, I give a rotation by 120 degrees, like in this way. So, about this axis, I give a rotation of 120 sorry 120degrees. So, what will happen? This, I will get again a triangle, because this is an equilateral triangle any rotation about this you know center of marks, center point if I given 120 degree rotation, then I will get again and equilateral triangle. So, here if I give you know rotation which is clockwise, then what will happen? This one earlier which was in the top, it will come now here, two will go here, and three will come here. Now if I had not have mark this hydrogen atoms, then I would have no option to figure out whether even has done anything with this atom, but actually you can take this atom and rotate it, suppose.

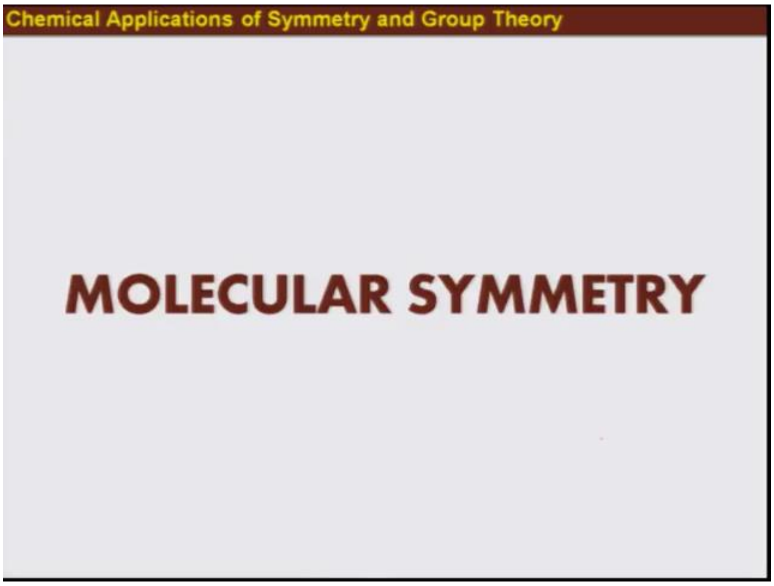
So, I can get several indistinguishable structures of these molecules. And if I ask you at this moment, you have seen water structure and you now, you are seeing the structure of ammonia, and we said water was symmetric ammonia is also symmetric, which one is more symmetric? The obvious answer will be ammonia, probably we have, you know started developing that, if by some means we can get more number of indistinguishable structures for a molecule, then the other, then the second molecule will be more symmetric, we will try to be more quantitative.

(Refer Slide Time: 19:59)



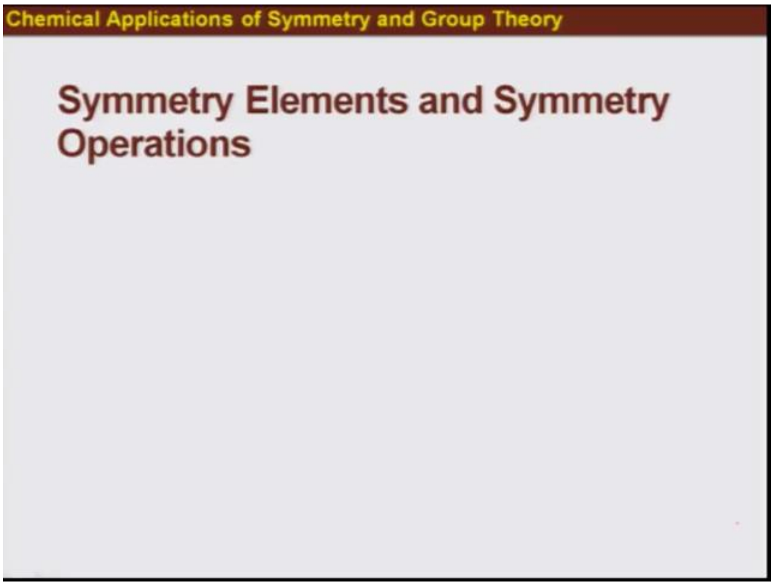
So, now we have Benzene in our picture. So, undoubtedly, anyone will say this is highly symmetric, that is what exactly one will used the term, highly symmetric, and this is way more symmetric than Ammonia an; obviously, than water. So, another molecule, methane, this one is also very symmetric.

(Refer Slide Time: 20:28)



Now, we will try to find out, how we can you know say that one particular molecule, molecular structure is more symmetric than other. So, as I said already that, you can have an intuition, by which you can say that this is symmetric, and this is more symmetric than other, but how you can be with more quantitative in that sense, can you use some mathematical tool, or mathematical you know, way to say exactly this particular molecule is more symmetric than this one. So, that is what we will try to do now.

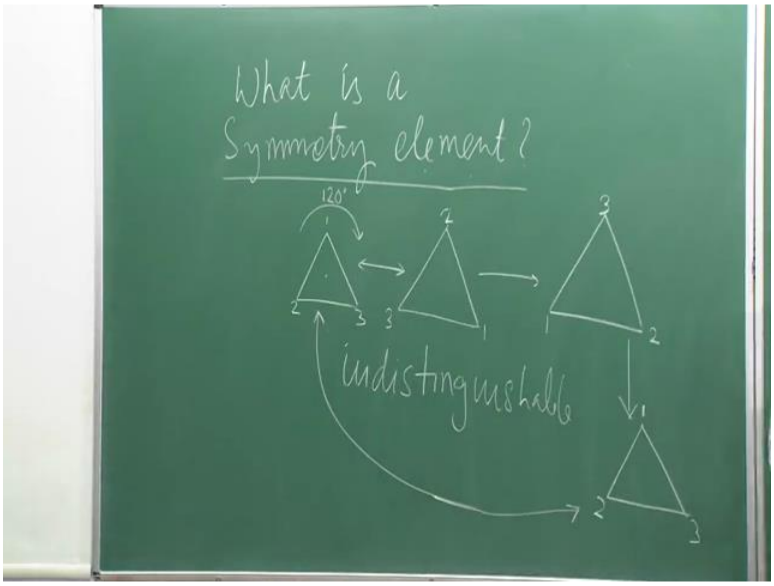
(Refer Slide Time: 21:16).



So, that is done by some concept of Symmetry Elements and symmetry operations in a molecule, and at the end we use this Symmetry Elements, and symmetry operations, to form a mathematical group. And this mathematical group is utilized to you know, quantify the symmetry aspects of a molecule, molecular electronic states, its wave functions, and so on, and which will be using throughout this course.

So, we have this two things, Symmetry Elements, and symmetry operations.

(Refer Slide Time: 22:07)



So, let us first worry about symmetry operations. So, what is a symmetry operation? So, let us, what is a symmetry operation that is our question. So, Symmetry Operation is, is a movement by which, any object can go from one, you know, configuration to an equivalent or identical even, configuration. So, when I say this equivalent, I can for sure use the term, that under this movement object goes from a particular configuration, to another indistinguishable conformation.

So, say for example, if I have an equilateral triangle, and I can imagine that there is an axis about this. So, the axis is toward you, the axis is out of the plane of the board, so if I given rotation about this. So, suppose I give a rotation like this, by 120 degree just like we showed earlier, I get another equilateral triangle, and these and these, this two are indistinguishable. Do not go by my trying, that will give you different size, but assume that this two or equilateral triangle of same size. So, this two are indistinguishable. So, we say indistinguishable structure. If I could mark, then I could write like, this 2, 3. So, upon a 120 degree rotation, this will come here, 1 comes here, and 2 goes here and; obviously, 3 comes here. So, this two when I mark them, I can say that they are indistinguishable, but they are not identical.

Now, if I give one more such rotation. So, then in that case, 2 will come here, 1 will go here, three will go here. So, I have are configuration like, 1 comes here, three goes here, 2 comes here, and another such rotation will give me a structure for which, 1 is going here, so, this is 1 2 comes here, three is here. Now you look at this, relation between this and this, they are identical. So, by doing something, by moving this body about this axis, by a certain angle that is 120 degree, I get an indistinguishable structure. Another rotation by same amount of angle, I get another indistinguishable, and then another rotation will give me back the identical structure. So, these movements by which I can get, you know, indistinguishable structures or even identical structures, are called Symmetry Operations. So, Symmetry Operations you know, it can be explained in another way also, that is suppose I am looking at some object, and then for a moment I turn around I am not looking at the object, now someone comes and does something goes away, and I turn back again looking at object, I cant figure out whether there is any change made on that object. Then what the person did when I was looking back is a Symmetry Operation. Now that is about symmetry operations. Now then what is Symmetry Element?

So, next question will be what is a Symmetry Element? Symmetry Element is, is some entity within the body, it can be an axis, it can be a point, it can be a plane. So, this axis or plane or point, about which a Symmetry Operation takes place, and we get and indistinguishable structure, is known as Symmetry Element, Symmetry Operations are done about the Symmetry Element. So, you can figure out that here, we were giving a rotation about this axis, the axis which is toward you. So, about this axis, I am doing a Symmetry Operation, which is called Rotation, and this is called, this axis is called a Symmetry Element (Refer Time: 28:04) rotational axis. We will talk about that in detail in the following classes alright? So, you can figure out that, Symmetry Operation and Symmetry Elements are very much, you know, interdependent, I mean, sometime you know this be can become bit confusing. So, you cannot have a Symmetry Operation without having a Symmetry Elements, and symmetry operations can be, you know, performed only when you have Symmetry Elements. So, when we try to tell that, any or particular object, or in is a molecules, one particular molecule has you know more symmetry than another molecule, then what we do is, we look at the symmetry operations and the Symmetry Elements of the molecules.

So, if a molecule has more number of Symmetry Elements and Symmetry Operations then; obviously, that object is called you know a more symmetry, then an object which has less number of Symmetry Elements and Symmetry Operations. So, if we just think about the structures that we showed that is, Benzene, Ammonia and water. Now if you think about those structures, then the conclusion based on whatever you have heard till now in this class, is that, Benzene which appears to be more symmetric, must have more numbers of Symmetry Elements, or more number of Symmetry Operations, than Ammonia, which in turn will have more number of Symmetry Elements, Symmetry Operations than water.

So, in the following class, we will know more about the specific Symmetry Elements and Symmetry Operations, how to find them out, and later on we will try to you know club them, in something called point group. So, we will see again in the next class, till then, have a good day.