Circular Dichroism and Mossbauer Spectroscopy for Chemists
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Lecture – 1
CD Spectroscopy

Welcome to this course of Circular Dichroism and Mossbauer Spectroscopy for chemist. My name is Arnab Dutta and I am an associate professor in the Chemistry Department of IIT Bombay. So, before we jump into the details of circular dichroism and mossbauer spectroscopy, we would like to know why should I know about these things and over here we will learn one important aspect that is known as symmetry.

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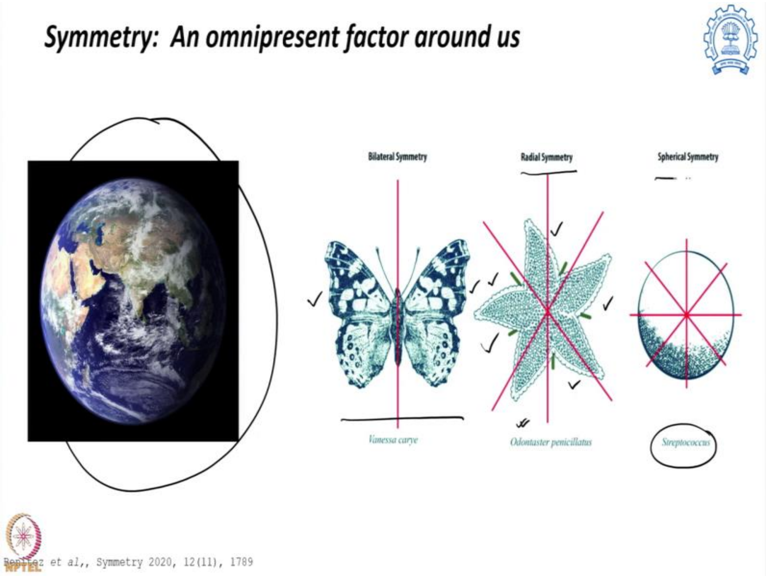

So, if we look the world around us. So, this is the blue planet we can see around us and over here we have multiple different variants of life forms. Although they are divergent in numbers there is one very unique thing among all of them, there some symmetry around them. So, what is symmetry? So, there are 3 examples. I am showing first is a butterfly. If you take a look, it tells to us there is something naturally mimicking over here.

So that one part of its wing matches the others and over here we call them as bilateral symmetry. We will talk a little bit more details on that in the coming minutes. Also, we see this particular sea creature where we can see there are different portion of this body are actually symmetric and if we go around this lines, we see a symmetric arrangement of that. This is called the radial symmetry and the last we also have spherical symmetry.

So, this is one of the examples of a bacteria which is showing over here. You can see, it is look a spherical in nature and that is also concentric from its center. So, we will call them as spherical symmetry. So, these are the 3 different symmetry we actually saw all around us whenever we look into the world. So, now we will go a little bit more details of this particular symmetry and describe each of them.

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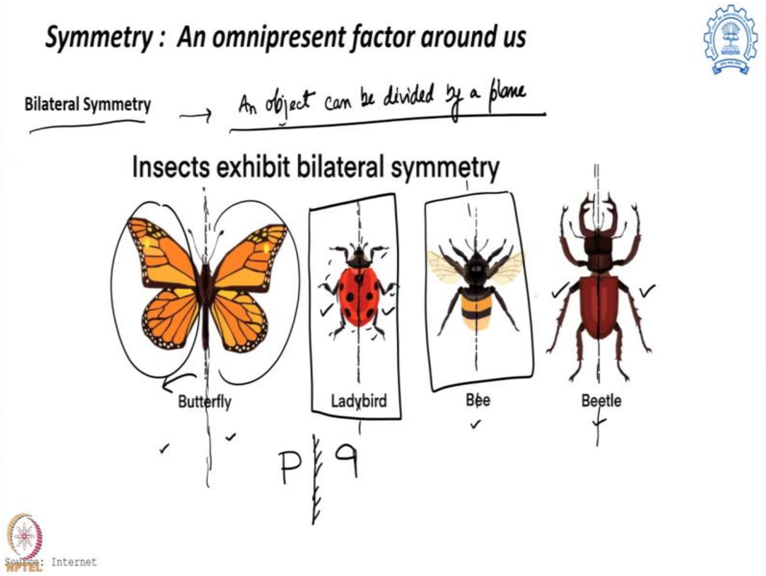

So, first let us try with bilateral symmetry. So, now, if I want to define what is a bilateral symmetry? So, bilateral symmetry is a symmetric when an object can be divided by a plane and on the other side of the plane, we see the similar parts. So, for an example, again we are bringing the butterfly and here is the plane. On this side of the plane, whatever we see its actually mirrored on the other side. So that is why we call them a bilateral symmetry.

So, there will be a plane and either side will be very similar. So, as you typically draw like, there is a mirror image over here. So, if I am drawing something over here say like P that will be mirror imaged on the other side, so that is known as the bilateral symmetry. Then we look into this ladybird again very similar to the butterfly you can see. If I draw the line along with this particular plane, both sides are same, including the shape of their legs number of their legs to the pattern on the system.

There is a bee, this is a beetle, we are following the same trend all over the place. So, there is a plane of symmetry on either side I am seeing the same thing. So, this is a bilateral symmetry which can be found in number of different life forms around the world and it is one of the most important symmetry that we observe around us. Then we go to the next one.

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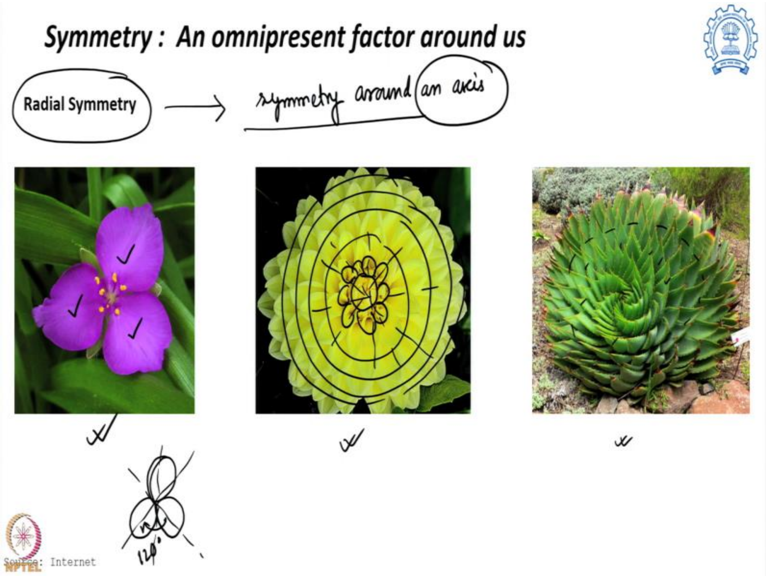

This is known as radial symmetry, so, what is radial symmetry? Over here we found the symmetry around axis. So, previously we are looking everything around a plane. Now we are looking around an axis. For example, let us take this first example of this flower. Over there we can see there are 3 different petals of that and they are symmetrically added such a way that along with the axis, if I rotate, you actually found a similar system.

So, if I draw the line we can see, the angle between them is actually 120 degree, so, this is the symmetry we have over here. The second flower, the symmetry, is a little bit more complex, but we can see it is still there compared to here. Once you go all around this petals, you can say they are symmetrically oriented around it and each of them actually distributed along a axis and this actually goes in different concentric circles and that is how this flower petals has been oriented.

So, it is a little bit more complex than the first flower but the basic template is actually remaining the same. The last one is actually a much more different one, but over here also we see a radial symmetry along with an axis. All these different portion of this particular tree is actually oriented. So, this particular plant have also an radial symmetry. So, other than bilateral symmetry where we see the symmetry around a plane.

In radial symmetry, it is around an axis that is the main difference and both of them are the major component of bringing symmetry around in the world.

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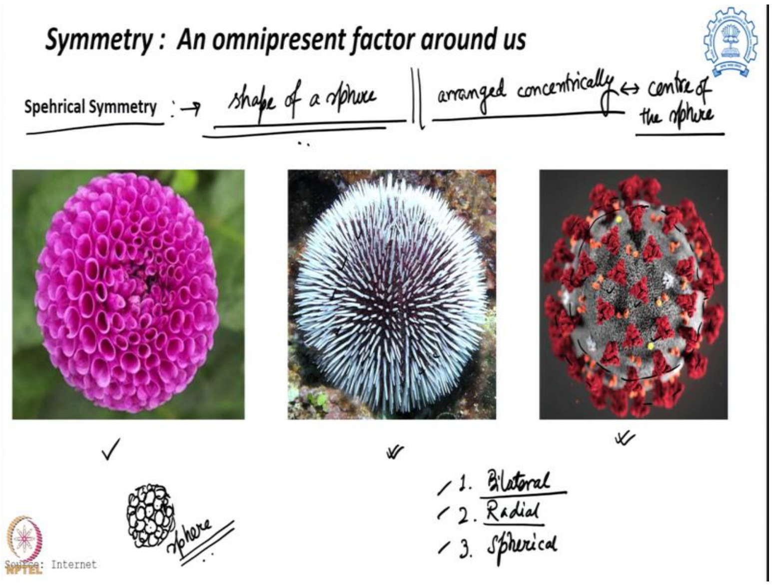

So, let us go to the last one, the spherical symmetry. What is spherical symmetry? Spherical symmetry is actually having. First, you have to have a shape of a sphere. That is the first thing you need and then all the other things around it will be arranged concentrically. So that there is a connection from the center of the sphere. So that is the basis of spherical symmetry.

So, over here for an example, we take this particular flower and over here you can see that the flower is actually oriented at first in a large portion which we can actually called a sphere and all these small petals are actually a little bit different than the radial symmetry we are discussing in the earlier segment. In the radial symmetry we are mostly remaining in one particular plane and over here in 3, dimensional orientation we are actually spreading around the sphere.

So, the presence of this spherical shape is actually bringing me the spherical symmetry and, along with that we have all these petals which are actually arranged in a particular orientation from the center of the circle. So that is why it is known as the spherical symmetry. This is the same thing, but in the form of a sea creature which is known as a sea arching. So that is actually having the same thing.

So, you can see all the different white portions coming out of it. It is actually oriented such a way that it is continuing to have the spherical shape and at the same time, it is connected from the center of the sphere in a proper way and this one, I think all of us know what it is after this covid 19 attack. It is the virus of that covid19 and you can see it is also having a spherical symmetry. The basic system, what we are having over here.

It is fear for sure, but all these proteins that is actually coming out of the system. Now we know of the name also when that the spike proteins, they are also oriented in a very much symmetric manner and it is actually maintaining the spherical symmetry. So that is why spherical symmetry is also one of the other large component of the symmetry that we see all around us. So, there are 3 different symmetries.

We want to just continue and over there one is the bilateral symmetry. One is the radial symmetry and the last one is the spherical symmetry.

So, these are the 3 important factors that we found. Bilateral is the symmetry around the plane. Radial is a symmetry around an axis and spherical symmetry you have to have a sphere first and then you have a concentric arrangement around the center of the sphere. So, these are the 3 major portions of the symmetry that we can come about.

Now let us go to the next one. Over here there is a another portion of the symmetry also coming to the picture and that is known as the chirality. So, what is chirality?

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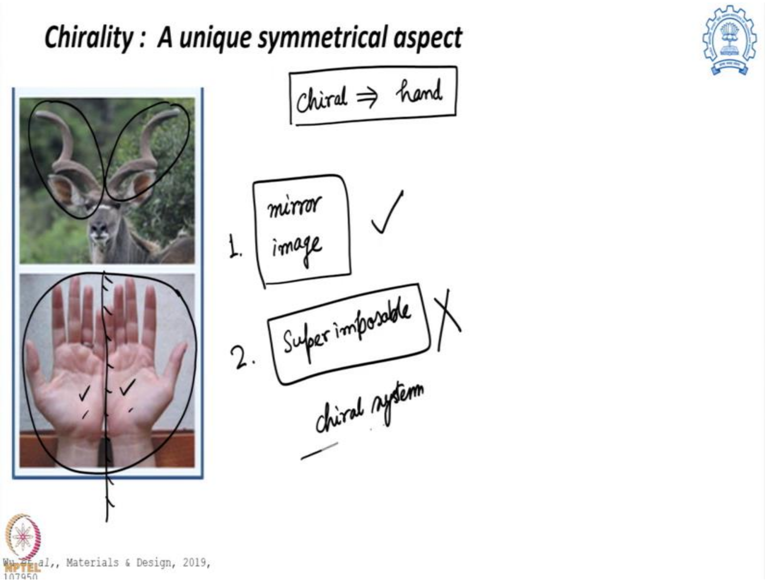

This term chiral is derived from a Greek term which means hand. So, chirality means handedness and this is actually coming from this particular picture. We are showing over here is from our hand. We can see that our hand is actually mirror image of each other, both the hands. So, if you put a mirror and put your hand, you see the exactly the same thing, their mirror image.

But despite being mirrored image, if you want to put the hands on top of each other, they do not match. For example, this hand is actually mirrored image of this, but if you want to put on the top of that you can see they are not really sitting on the top of it. So, which is called they are not super impossible or indistinguishable. So, this particular system is known as the chiral system, where I have the mirrored image of each other, but they are not super impossible.

And over here you can see the horns of this particular deer actually having the same thing, they are actually mirrored image of each other. But if you want to put them on top of each other, they do not really fit on top of it and that is known as the chirality. So, chirality means mirror image of each other. But that is the first factor and the second factor is, they are not super impossible.

They are mirror image, but not super impossible and if the two criteria are actually maintained, you can say I have a chiral system and this chirality is also found quite often in biology.

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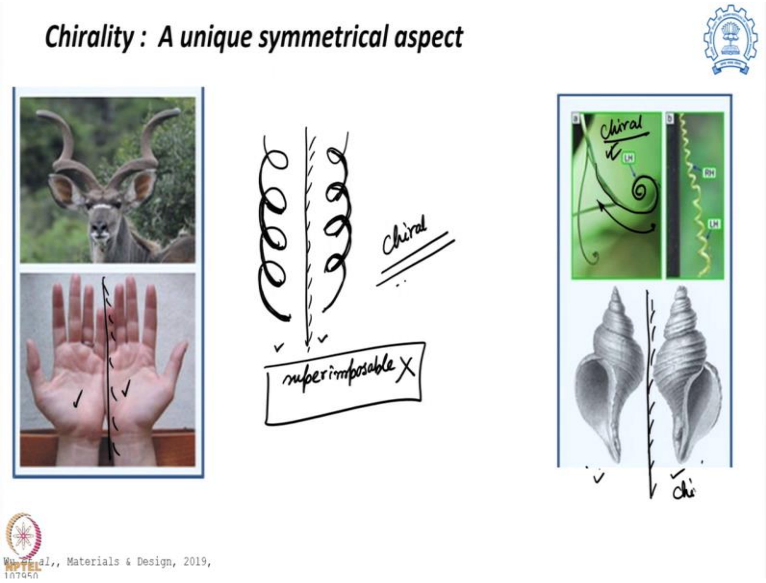

If I want to take another look into it. So, this is another one, so, this is, you can see a part of a newly growing leaf is coming out and you can see it is nicely making this kind of ring and this is this new segment is actually growing up. It is actually such a system that if you can take a mirror image of it and try to point on top of it. It is not going to be super impossible. So that means this is also chiral in nature over here also the spring kind of system.

So, if you have a system like this, so, it is moving like that. So, this is the front segment you can see this coming out and this particular system is rotating. How it is rotating and if I want to take a mirror image of it. So, this is a segment of mirror image and what we are going to see it is going to be the exactly opposite. That is how it is going to look like and you can see over here this is actually mirror image but they are not super impossible.

So that is why this kind of systems are also remaining chiral in nature. So, this kind of systems are also kind in nature which is matching very much similar to our hands which is mirror image of each other, but not super impossible and this is also skunk which is also showing the similar kind of motion. It is mirror image of each other but really not super impossible on each other that means this is also chiral in nature. So that is what we are finding in system a lot of chirality but why do we care about chirality?

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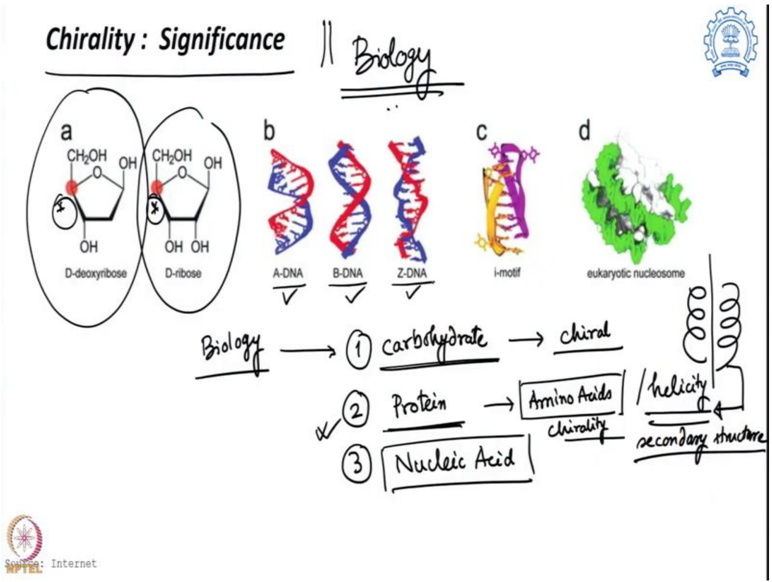

So, chirality is very much important in biology because biology uses chirality as an identity. So, for an example over here, I am showing you some examples in biology. If I take a look into it, what are the major components of the formation of the biological systems? One of them is carbohydrate, one of them is protein and one of them is nucleic acid. So, you can all agree these are the 3 major pillars of formation of a biological system from a very small one to a very large one.

And over here, if we look very closely, you can see this carbohydrate over here I saw if you look into the molecules of carbohydrate, they are actually having some carbon center such that they are chiral in nature. That means there are certain carbon centers such that they actually create a mirrored image that is not superimposable of each other. So that means carbohydrate actually is majorly chiral what is actually present in the biology?

Similarly, proteins is made out of amino acids and will go into the details of each of the amino acids that is naturally can be found in biology and over here that we found that almost all the amino acid, except one that is found. Naturally, they are chiral in nature, so, obviously, when the proteins are made out of this chiral amino acid, the system will be also chiral.

And at the same time, proteins also create secondary structure which also has their own chirality coming into the picture, especially the helicity. The Helicity is the thing that we shown earlier this kind of systems that we shown, so, this kind of helicity can be also bought in the protein by the secondary structure. So, this amino acids brings chirality and the secondary structure brings additional chirality to the system.

So, with that our protein system becomes guided and last, but not the least, the nucleic acid. So, these are the structure of the nucleic acid and we all heard about this how this double helix bundle of the DNA is formed and depending on how they are actually forming in the 3 dimensional space? We can divide them in these 3 major versions, A B and Z DNA and over here what we found this nucleic acid and it is quite obvious from the structure over there.

They also contains helicity and once you have helicity you will have a chirality because once you have a helix, it is right hand, helix or left hand helix these things will come out in the picture and once they come out, you have a system which is going to be chiral. So, in biology, you have all these simple systems, the carbohydrate, the protein, the nucleic acid, from the very basic to the larger portion.

They are actually maintaining the chirality and this chirality becomes the template of their molecular recognition because in biology, carbohydrate, protein and DNA play together to interact and they actually talk to each other among themselves. Through this molecular recognition and chirality becomes one of the most important factor of this molecular recognition and in the later portion of the class, we will cover some of the examples that how biology actually uses this chirality.

But over here our main goal is to find out. Yes, chirality is important in biology other than biology. We are also using a huge number of organic molecules that we actually create by our own non-natural ones and over there, this synthetic molecules also can have chirality.

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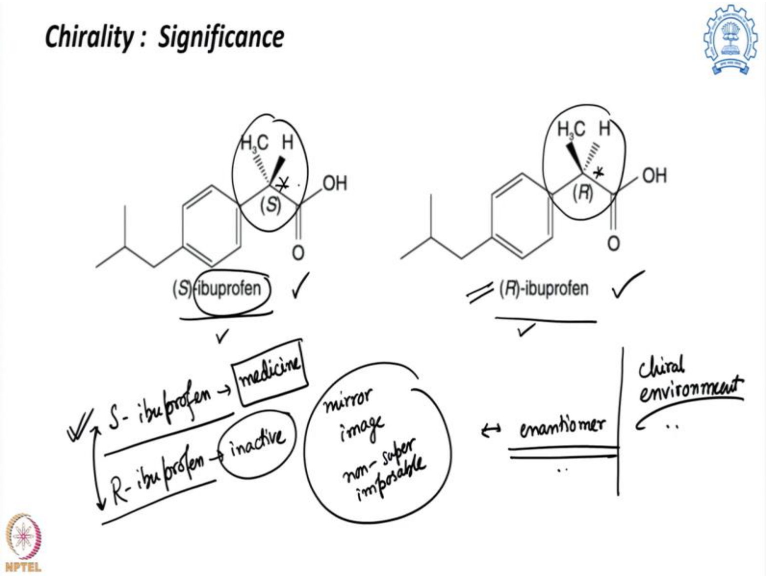

So, for example, over there, this molecule I have drawn. And most of you probably heard this name all together ibuprofen which is one of the most popular drugs at this moment and we are using it at a quite a high amount. This molecule is actually chiral because it actually has a chiral center and because it has a chiral center, it can have two different isomers, mirror image of each other and this mirror image are called enantiomers.

So, the mirror image which are actually non super impossible. They are actually known as the enantiomer and these 2 enantiomer, although their physical properties are very simple, but in a chiral environment they can be different. We have to remember that we can have these 2 enantiomer where there all the other physical properties might be exactly same. Their appearance boiling point they can be actually same.

However, the properties which requires the chiral environment then they actually separate themselves out. So, in a condition where I can induce chirality, they will differentiate between these 2 enantiomers of ibuprofen and that exactly happens when we actually put them in a biological system say during our body. So, when we consume this ibuprofen, these 2 are actually recognized differently.

The first ibuprofen, the S one, the S ibuprofen is actually has the medicinal quality. So, we can use that as medicine. So, if I take S ibuprofen, I will be fine because that will be going to work as an analgesic as it is supposed to do. But if I take R ibuprofen, although the structure is pretty much same except the orientation around this carbon center, this r ibuprofen is actually inactive in nature.

So, if I in take it, this is not going to show any medicinal properties so that much difference is actually happening between these 2 different enantiomer S and R. S is a medicine. R is remaining an inactive system and this difference is coming because of their chirality and recognition of their chirality in a chiral environment, a biological system like inside our body.

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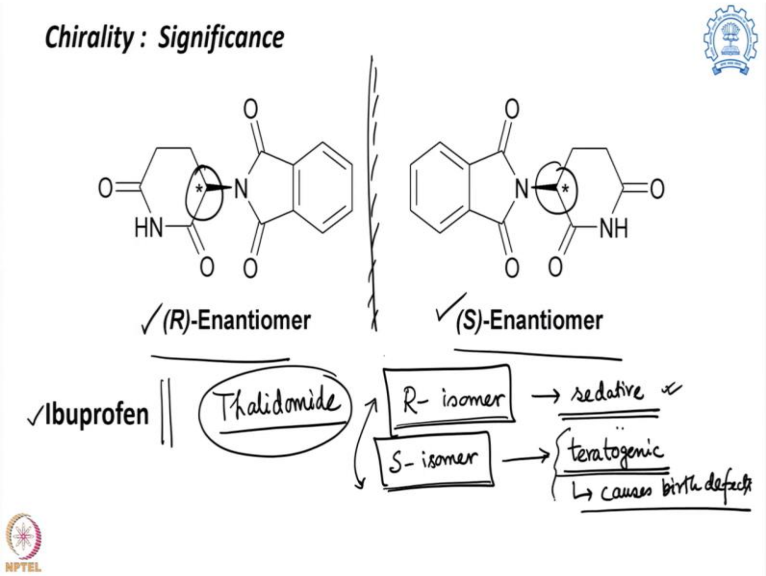

Let us take an another example of a system, so, we have already discussed ibuprofen. Now we are discussing an another molecule. This particular set of molecules the known name is thalidomide, so, these are the 2 structures of thalidomide. Again, we have a chiral center over here which actually are the mirror image, so, these 2 are actually mirror image of each other and then we reorient it to showcase in this particular way.

But this is the r isomer. This is the s isomer and this thalidomide can be also used as a drug. So, if we take the r isomer of the thalidomide, the r isomer of the thalidomide is actually act as a sedative. That means it can be used as a medicine, it has medicinal properties. However, if I take the r isomer by mistake, then it is an issue because previously what we found that one of the ibuprofen is medicine, the other one is inactive.

But in this case one is medicine, but the other one is actually little bit of problematic molecule which is known in medical term as teratogenic which means the presence of this particular molecule causes birth defects. So, you can say these 2 systems are kind of the story of a twin and one of them is evil. One of them is good, so, you have to be very careful that which of them we are actually consuming because one of them is a life-saving drug.

The other one is going to create a lot of problem so that we have to keep in mind and this is the thalidomide we have discussed.

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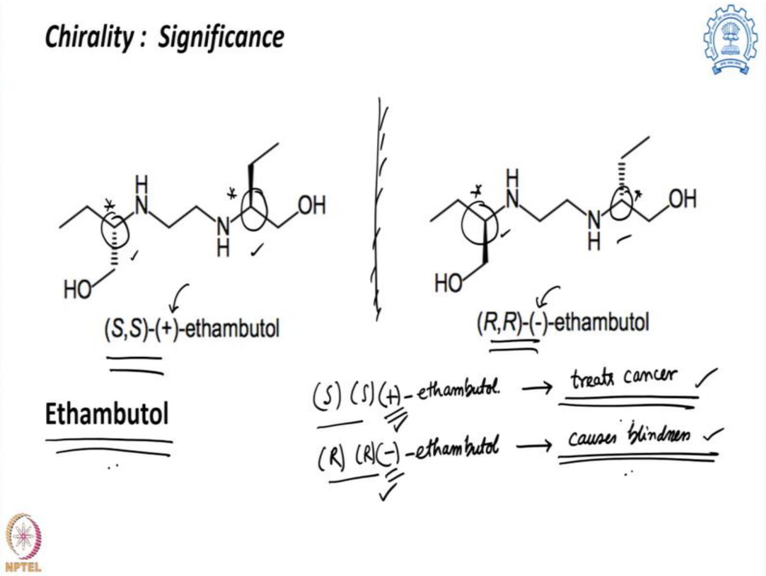

And then the last one we want to discuss is ethambutol. This is an another drug and over here you can see this is the structure of the molecule and over here we have 2 chiral center present in this molecule and this is the mirrored image of the molecule and over here these are the 2 centers and you can say this is actually replicating the structure but changing the orientation in around both the centers.

So, this one is the S,S ethambutol. This is the R,R ethambutol and then what are their properties? The S,S one is actually having a medicinal property. This actually treats cancer, so that means it can be a life saving drug whereas on the other side, the R,R ethambutol one actually problematic in nature that actually causes blindness. So, again we have to be very careful which of them we are actually consuming.

If it is SS form, it is the drug. It is the RR form it is going to be toxic to our system. So that we have to be careful of and over here I want to take your attention to the signs plus or minus. So, this plus or minus defines like, if I take this molecule which are chiral and put that in presence of a plane, polarized light which particular direction the plane polarized light is going to shift the positive side or negative side.

So, this is an experimental parameter that is actually can be measured for each of this molecules and why it is interacting with the plane polarized light? And how it is moving? We will discuss that in the coming days.

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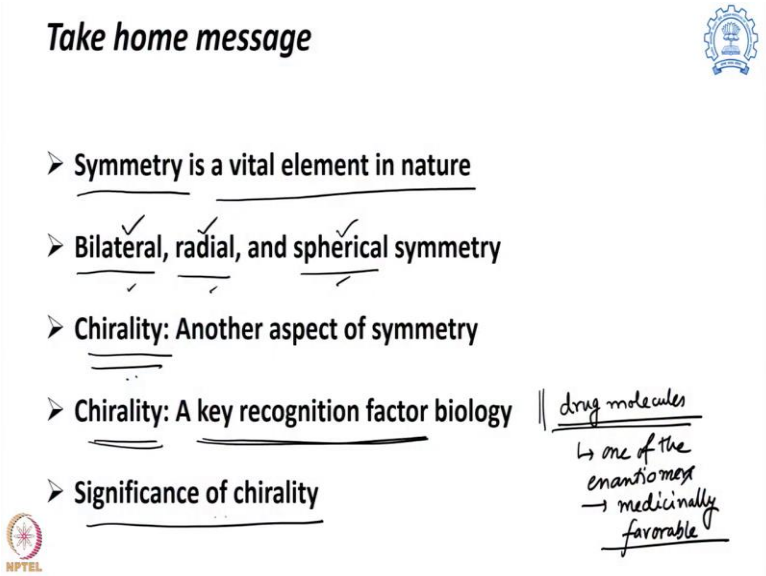

So, with that we would like to conclude this first session and over here, I hope that I am able to convince you that the symmetry is actually a very important aspect in nature and it is present in all different parts of the nature, especially in the biological form. And we found there are 3 different and Significant portions of symmetry, bilateral where the symmetries around a plane.

Radial symmetry around an axis and spherical where the symmetry originates from a spherical structure and remain concentric around the center and it is showing the symmetry. So, these are the 3 different aspects of the symmetry. We can see we find chirality one very important aspect of the symmetry where we are having a mirror image of a system which is not really superimposable and indistinguishable of the original one.

So that is known as the chirality and then we found this chirality is very important for the biology, because most of the biological template that is actually made out of the building blocks the proteins, the carbohydrate, the nucleic acid. All of them contains chirality and those calories. Also coming some of them from the helicity and those are actually a key factor, a key factor for molecular recognition.

And that is why we are very much interested to know about the chirality. And we have also shown some of the drug molecules which are chiral in nature and not only that only one of the enantiomers is actually medicinally active. I would say medicinally, favorable and the other form can be inactive and can also be toxic to ourselves. So that is why we have to know very well which particular enantiomer I am using.

And for that we need to have some experiment and have to know about the details of the chirality and that is why we need to know about chirality. So, with that we like to conclude this particular first segment on the chirality over here. Thank you. Thank you very much.