Symmetry, Stereochemistry and Applications
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Module No # 03
Lecture No # 15
Isomerism and Representation of Isomers

Welcome back to the course on symmetry, stereochemistry and applications. In the previous lecture, we have discussed about the various conformational aspects related to cyclohexane and substituted cyclohexane molecules. So now, we would like to move to the next part of this course which is to talk about the aspects of isomerism.

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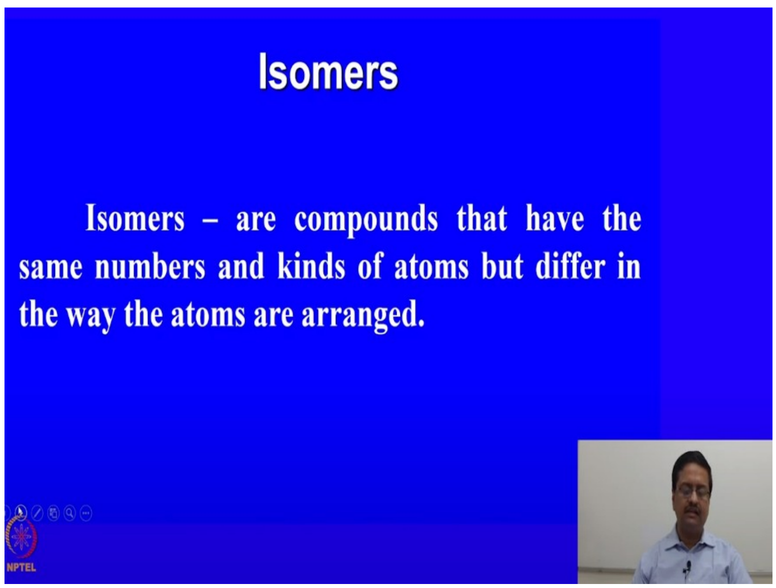

And how to represent it with isomers using the projection formula and significance. We all know that isomers are compounds that have the same numbers and kinds of atoms but different in the way the atoms are arranged.

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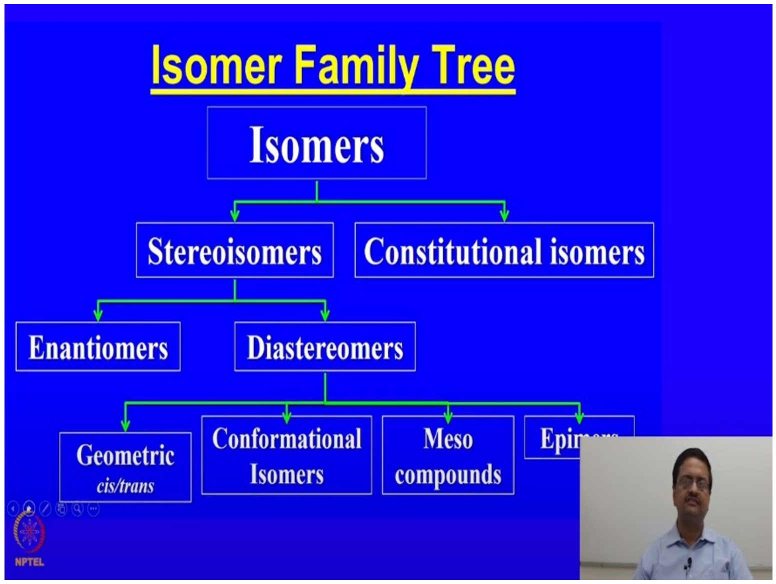

So let us try to see what are the different; types of isomer that are known. Isomers are specifically divided into 2 parts, stereoisomers and constitutional isomers. Stereoisomers are further sub divided into 2 parts, enantiomer and diastereomers and then the diastereomers are again further classified into 4 sections, which are geometric isomers or cis trans isomers, conformational isomer, meso compounds and the epimers. So we will slowly learn about all these different classification of isomers through this lectures.

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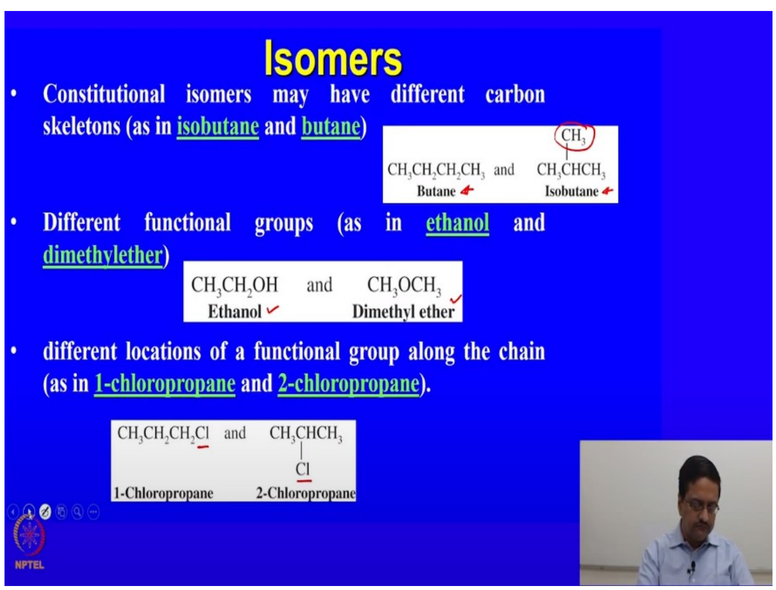

So when we try to first understand what type are the constitutional isomers we should know that constitutional isomers may have different carbon skeletons. That means they have the molecular formula same but may have it different carbon skeletons as is shown here in this particular example where you can have butane in a chain or linear form or the butane having a branch using a methyl group and forming as isobutane. So that is a constitutional isomer.

A different functional group may give rise to isomerism for example we all know in case of ethanol and dimethyl ether both of them have the same chemical formula C2H6O but the way the atoms are bonded are different in these 2 molecules are those are 2 different types of isomers of the same chemical formula. The third type of constitutional isomer can be different locations of a functional group or any substitution. For example here it is 1-chloropropane and 2-chloropropane that is the position of chlorine atoms is different in this 2 different molecules.

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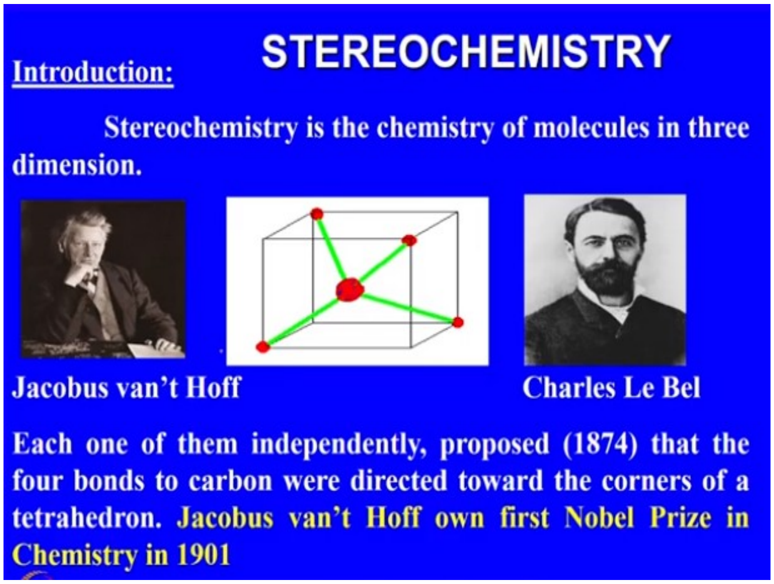

Stereochemistry was introduced more than 100 years ago. Stereochemistry is the chemistry of molecules in 3 dimensions. So we try to learn these orientations of atoms around a carbon atom. And based on that those orientations we try to understand different reactions and reaction mechanism which we will be discussed in the next part of this course. In 1874 Jacobus Van't Hoff and Charles Le Bel independently proposed that the carbon atom will have 4 bonds in tetrahedral orientation.

So for example if I have a carbon atom at the center and it is the 4 bonds will form a tetrahedron. And this tetrahedron is drawn inside the cube then it looks like this whatever is shown here. So this is the central atom which is the central carbon atom and the other four are its substituents which form the corners of a cube.

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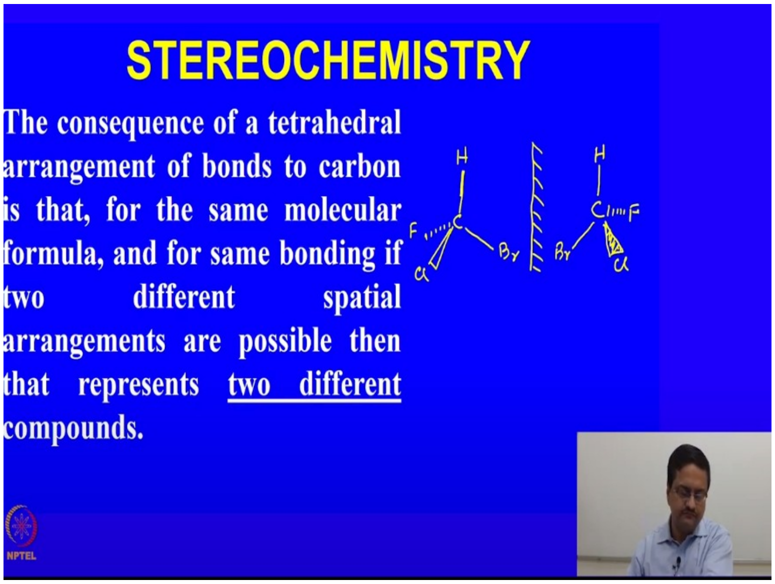

So the consequence of a tetrahedral arrangement of bonds of carbon is that, for the same molecular formula, and for same bonding if 2 different spatial arrangements are possible then those 2 different orientations or different arrangements are 2 different compounds. So for example I have 2 molecules here, so I have 2 molecules here formed by 4 different groups. So if you look at these 2 molecules, these two molecules are same because they can be super imposed on one another.

But if I do a replacement of one pair of bonds and connect them in a different way then, these 2 molecules will be different. What we see here these 2 molecules are now mirror image of one another. The blue and blue are mirror, red and red is a mirror, purple and purple is a mirror and the hydrogen is also at a mirror position or mirror images related. So therefore 2 molecules having same set of groups but arranged in a different way will result into 2 different compounds.

So the way we draw that in 2 dimensions is this. Suppose I have hydrogen here connected to carbon and a bromine atom connected to carbon like this then I can have two other groups above the plane of projection may be a chlorine atom and below the plane may be the fluorine atom. So if I draw the mirror image here this hydrogen is connected to this carbon atom, the carbon atom is then connected to the bromine which is the plane of the board.

And then I have 2 groups which are chlorine above the plane of the board and the fluorine which is below the plane of the board. And these 2 molecules that we have here are mirror image of one another and they cannot be super imposed on one atom. If I try to super impose then white goes with white and red goes with red but the blue and the violet they do not go one on another. So this two are not super imposable and they are mirror image compound. So these two although have same chemical formula are 2 different compounds.

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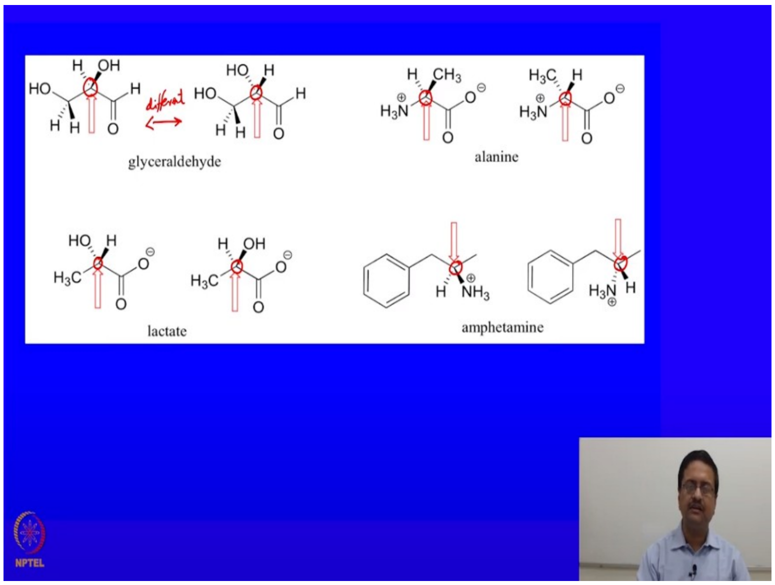

So like that when you have 4 different groups connected to a central carbon atom then we give rise to the center which is called the chiral center. So here in these few molecules which we have shown if you look at this carefully, at these bond which is shown as with the arrow this point, we have 4 atoms and the way those OH group and hydrogen atoms is connected to that are different. So these 2 compounds are 2 different compounds.

Similarly here also at this center the methyl and hydrogen atoms are connected in different ways. In the first case, the methyl is above the plane of the projection. While in the other case the methyl is below the plane of projection, as a result it gives the 2 different forms of alanine. The same is seen here and as well the same is seen here. So this gives rise to different compounds if you have different ways of attaching the group to a central carbon atom.

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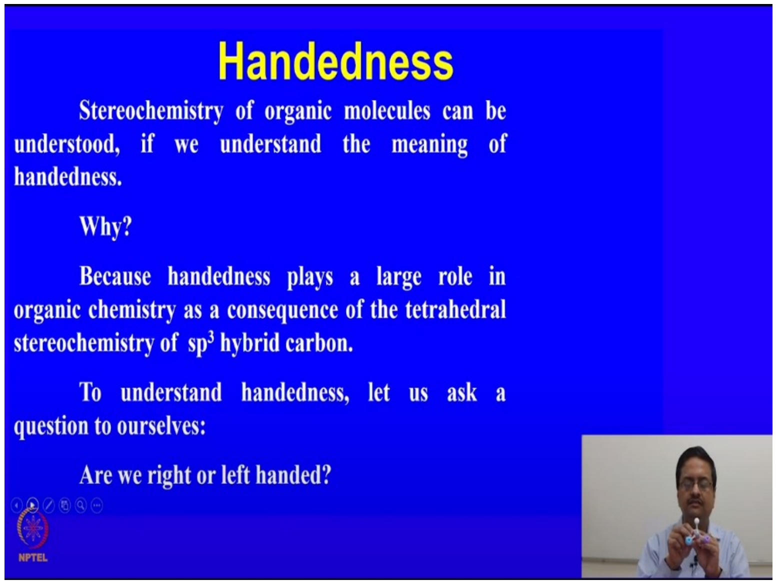

So the stereochemistry of organic molecules can be understood, if we understand the meaning of handedness, why? Because the handedness plays a role in organic chemistry as a consequence of tetrahedral arrangement of sp3 carbon. Sp3 carbon has four atoms connected like that and these 4 atoms can be connected to that central atoms in 2 different ways, either this blue atom on the right and this atom on left or the reverse.

So with respect to you it is left and right and I can have it right or left. Keeping hydrogen and this red atom as it is keeping the hydrogen up and red pointing towards me.

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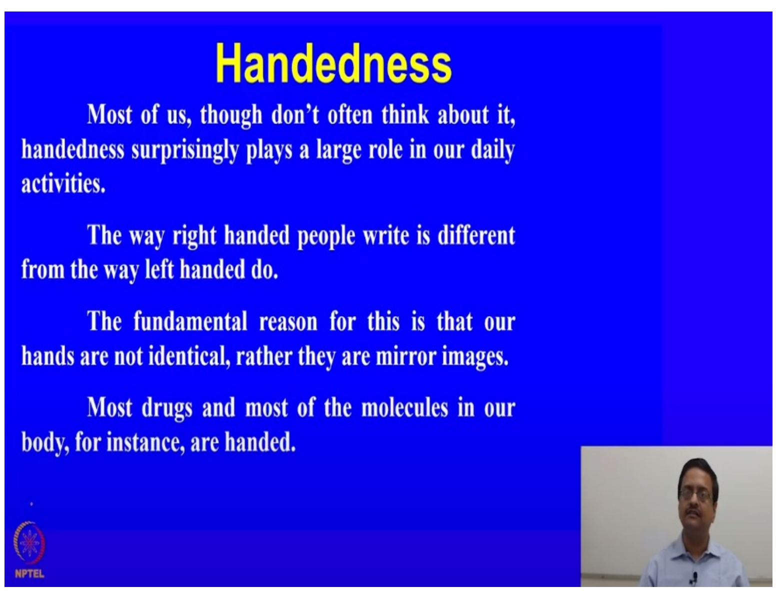

So when we try to see this handedness we try to see the way the right handed people write and with the left handed people write will be difference. For right handed people we write like that and the left handed people would write like this. The fundamental reason for this is that our hands are not identical rather they are mirror image of one another. So most drugs and the most of the molecules in our body are handed that means they are mirror image of one another.

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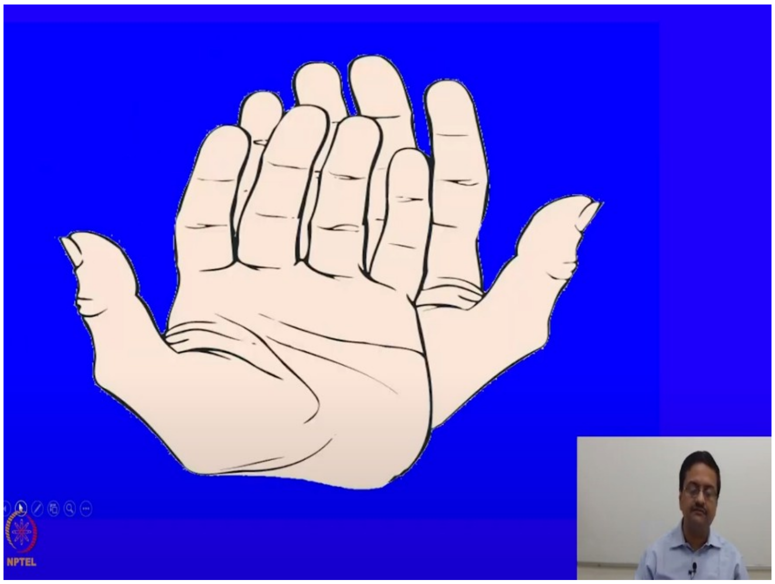

See you are I am trying to show this screen is the image of 2 hands like this. And those 2 hands are the mirror image of one another like this and when you try to super impose one on the other you cannot do that because those 2 are different in their handedness. So one is right hand and the other is left hand and when the figures try to match the 2 thumbs point 2 different directions.

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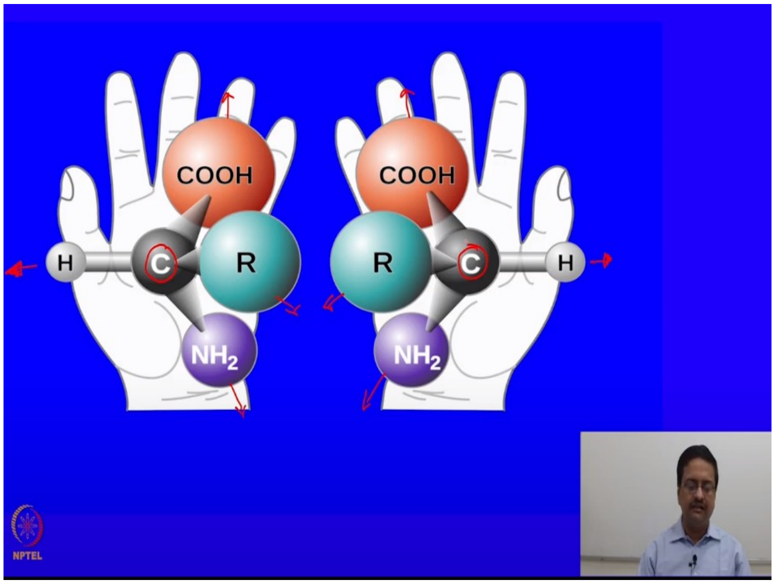

So therefore these 2 hands are different and these different is manifested in 4 bonds of carbon atoms which are responsible to give rise to different geometries around that central carbon atom. So here in this particular example you can easily identify that the carboxylic acid group is up in both the cases. NH2 group is down in both the cases, the R group is pointing towards us in both the cases. But the hydrogen here is pointing toward left and here the hydrogen is pointing towards right.

So this means these 2 molecules are different and the arrangement of those atoms about this central carbon is different. So this difference in orientation of the bonds make these 2 molecules are completely different. So it will have difference physical properties.

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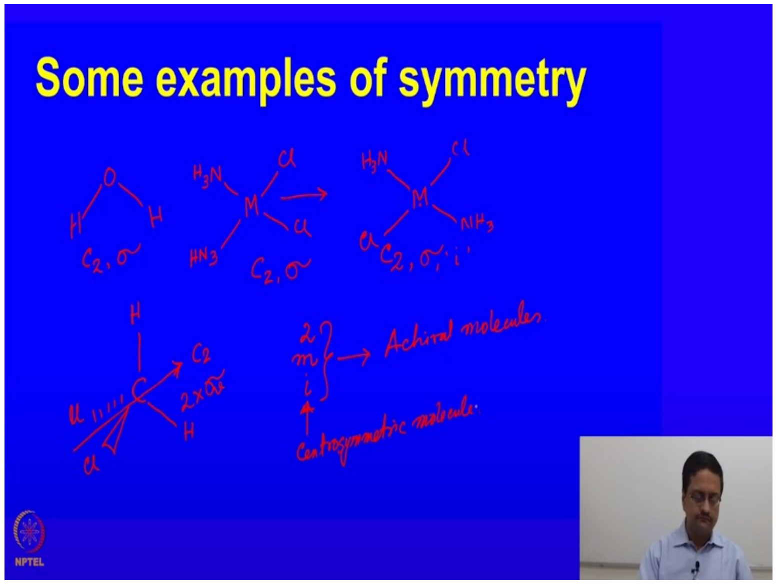

So when we try to understand the presence of chirality we try to understand the presence of asymmtery molecule we should also reconsider or understanding or presence of symmetry in the molecule. See for example a molecule which is suppose water has a 2-fold symmetry or a C2 axis and has sigma planes mirror planes. Similarly if I have a metal complex with 2 groups like this, 2 groups here, this molecule also has, C2 axis and sigma planes.

There may be a molecule like this where you have a metal bonded to 2 chlorine has trans and 2 ammonia as trans. This molecule also has a different symmetry what all we have here is a 2 fold axis that is a C2 axis, a sigma plane and the inversion center i, located at the center of the metal atom. Similarly if you try to draw a carbon based molecule like this where we have 2, hydrogens like that, and 2 chlorines like this which is nothing but dichloromethane a very well-known solvent.

This molecule will also as a C2 and 2 numbers of sigma Vs. So when any molecule has this kind of symmetry elements either the 2 fold axis or a mirror plane or an inversion center. These molecules are termed as achiral molecules. The molecule containing i is called as centro-symmetric molecule.

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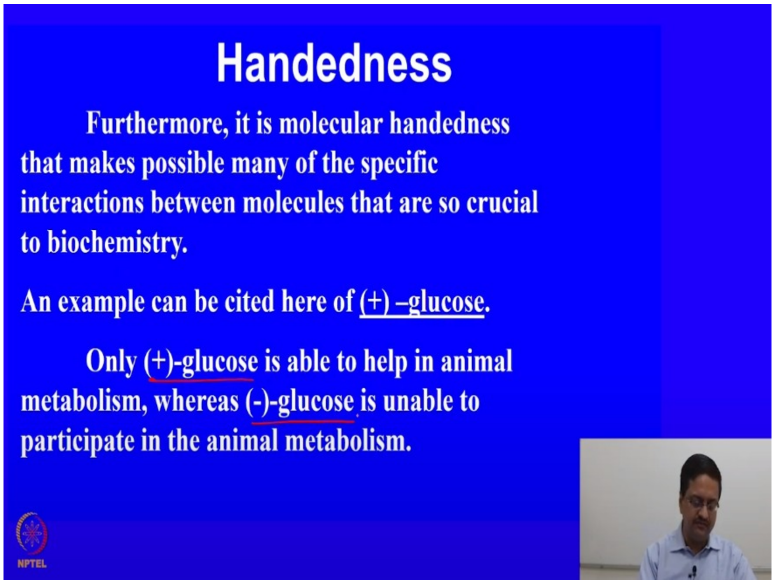

So it is the molecular handedness that makes possible many of the specific interaction between molecules that are very crucial in biochemistry. So some of the handed molecules are biologically active and some opposite handedness molecules are biologically inactive or not active as the other one. So for example + glucose can be cited here. Only plus glucose is able to help in animal metabolism, whereas minus glucose is unable to participate in the animal metabolism process.

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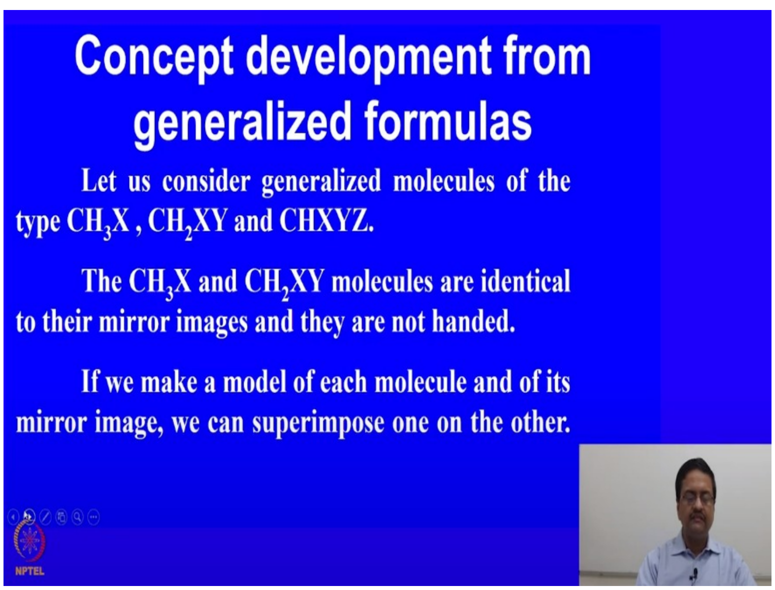

So when we try to understand the origin of this chirality. We consider 3 different generalized molecules CH3X, CH2XY and CHXYZ. So what we see that CH3X and CH2XY molecules are identical to their mirror images and hence they are not handed set of molecules. If we make a model of each molecule and its mirror image we can super impose one on the other.

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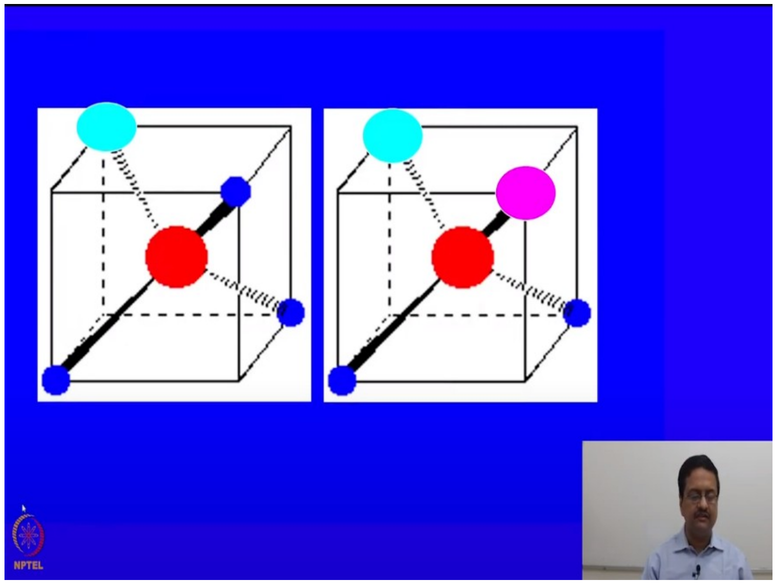

So for example if we have this molecule where you have 3 groups same and where you have 2 groups same. You take a mirror image of this molecule you will see that the mirror image can be super imposed on the original molecule without any problem. Therefore these molecules are not handed or not chiral.

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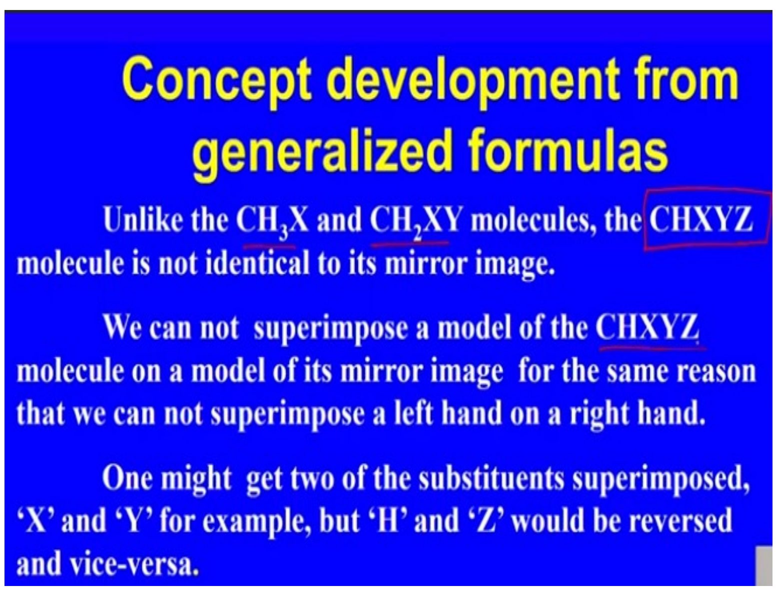

But unlike CH3X and CH2XY if we have a new molecule where all the 4 groups are different the molecule is not identical to its mirror image. So we cannot super impose the model of

CHXYZ molecule on a model of its mirror image for the same reason that we cannot superimpose a left hand on right hand.

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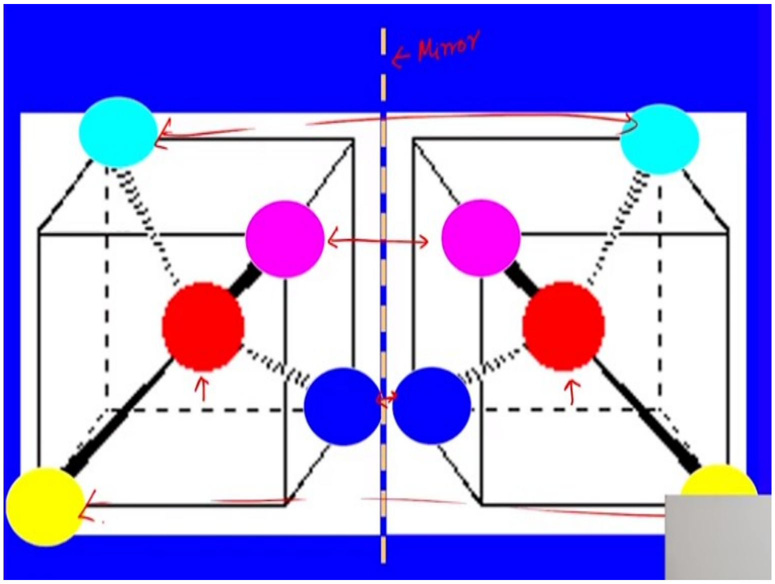

So let us see this by doing a mirror image relationship. So, on the left hand side we see a tetrahedral carbon at the center with 4 groups difference and here we have a mirror. So the mirror generates mirror image on the right hand side and that mirror image reflects one to one. But this 2 compounds are non-super impossible and as a result these 2 are stereoisomers or these two are 2 different enantiomers.

So this is how you should try to understand here that these 2 molecules that I have shown you before, these 2 molecules are mirror image of one another right. Blue and blue and red and red and purple and purple with the hydrogen on top, but these two to try to super impose one another they cannot be super impose only 2 atoms hydrogen and the red atom or the oxygen atom are super imposed and the other 2 atoms are not super impose.

So these 2 atoms are not super imposable mirror images of the same of the same compound. So they are two different compounds.

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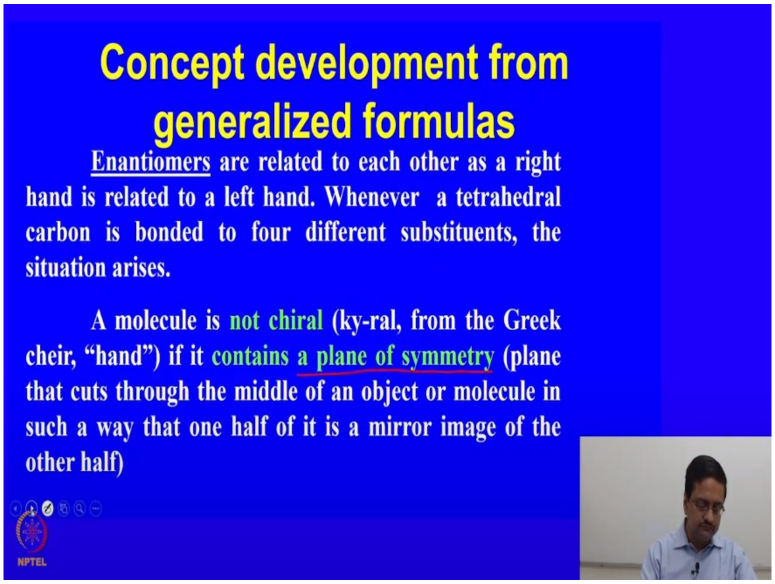

So we define enantiomers as enantiomers are related to each other as a right hand is related to left hand. Whenever a tetrahedral carbon is bonded to 4 different substituents the situation arises. So a molecule is not chiral if it contains a plane of symmetry which is very important. A plane of symmetry that cuts through the molecule into 2 parts and those 2 parts are mirror image of the other half. As a result that molecule cannot be a chiral molecule.

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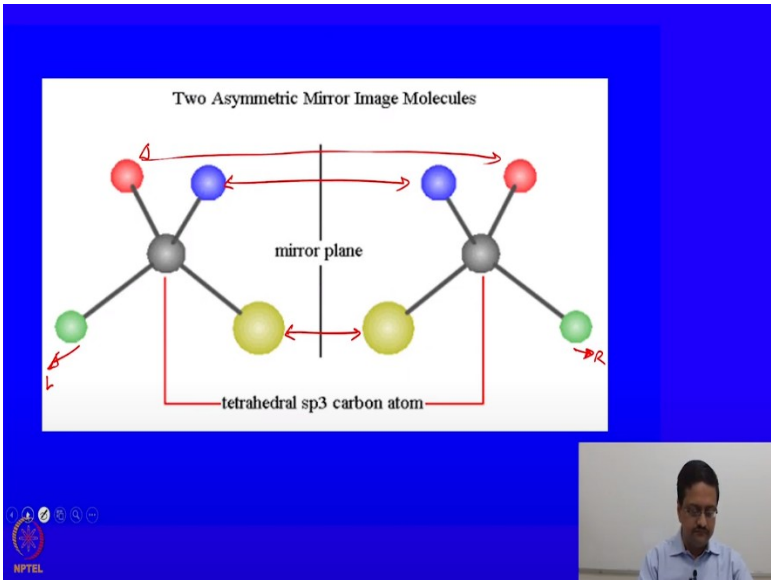

So here again I am showing you the pictorial manner how these 2 molecules are different, 2 asymmetric atoms 2 mirror images represent here that the molecule that are related are like this and this green atoms are pointed towards the left whereas the green atom here is pointed towards the right. So as a result these 2 molecules are different.

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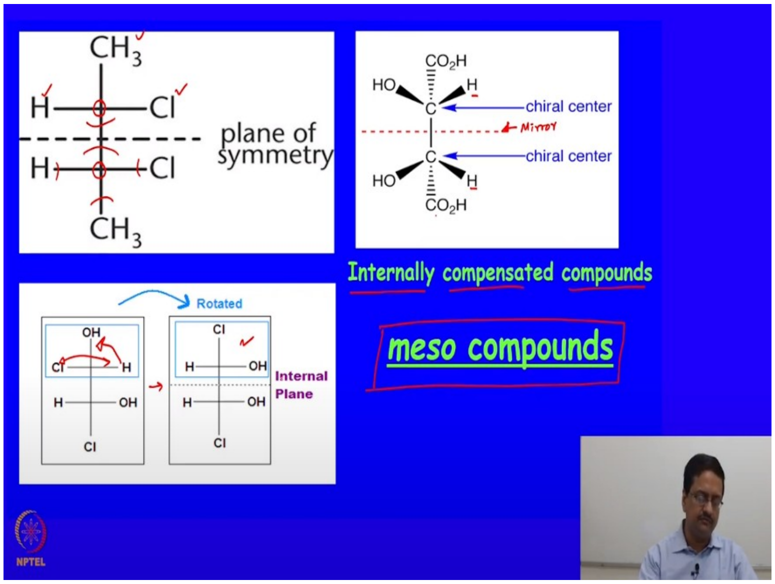

Now if you look at this particular case where I have 2 centers where both the centers have 4 different groups attached, here I have hydrogen, chlorine, methyl and a large group attached to this. And similarly on this, I have hydrogen, chlorine, methyl and a large group attached to that. And both the carbons centers are chiral but overall the molecule has a plane of symmetry, the molecule has a mirror plane.

And therefore the molecule is not a chiral molecule. So this type of molecules are called the internal compensative compound or the meso compounds. You see this other 2 examples where I have carboxylic acids on top and bottom, OH groups on the left hand side and the hydrogen on the right hand side. And this dashed line is a mirror plane which actually reflects the top portion of the molecule to the bottom portion of molecule. And hence this compound is again not a chiral molecule.

If you look at this molecule here, what we have done in this molecule is that you have made 2 changes. First we have changed the position of chlorine methyl hydrogen and then we have made the change between the chlorine and OH and made this molecule. So these 2 changes made the molecule look like this and it has again a mirror plane here. So these 2 changes made the molecule look like that it has internal plane of symmetry. So therefore this also a meso compounds.

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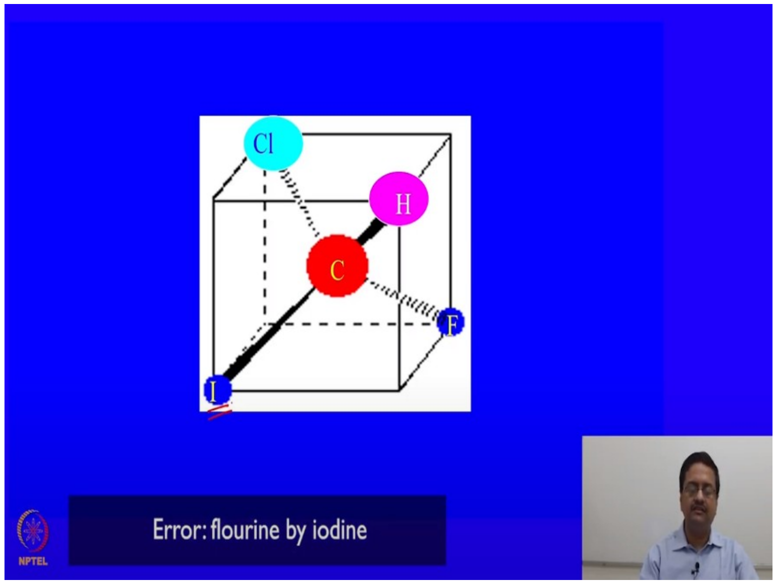

Here in this particular example you see that this particular compound has 2 group same and this 2 group being same the compound has a mirror plane. And, that mirror plane, presence of mirror plane makes this compound as an achiral molecule. But if I replace the fluorine one of the fluorine by hydrogen the mirror plane disappears and hence makes this molecule as a chiral molecule.

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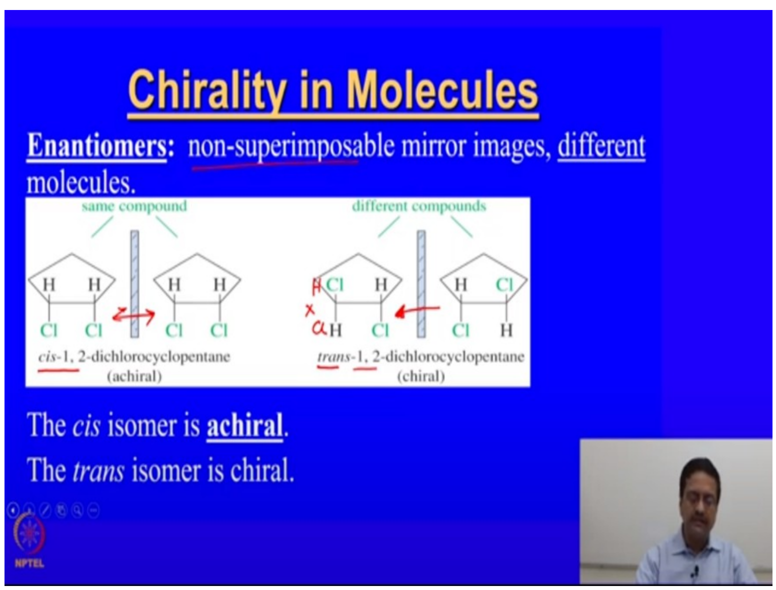

Let us see in another example that how the orientation of arrangement of molecules make one compound chiral and a different orientation makes it as achiral. As we know that enantiomers are non-super imposable mirror image relations and they are different molecules. Here we have taken the example of this 1,2 dichlorocyclopentane. Here what we see is that this compound and that compound, that they are mirror image.

And these 2 mirror images can be super impose on one another. Therefore these 2 compounds one at the same. But here what we have done is in case of trans 1,2 dichlorocyclopentane the mirror image looks like this and when you try to bring this mirror image and try to super impose on the original one this chlorine will fall a super imposition with the hydrogen. And that hydrogen will try to super impose with chlorine and that does not give you a correct super imposition.

So therefore this compound and its mirror image are 2 different compounds. And that is why we can consider that this trans 1, 2 dichlorocyclopentane is chiral molecule. So we end this session here and in the next session we will start learning about Fischer projections. Thank you.