Symmetry, Stereochemistry and Applications
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Module No # 05
Lecture No # 23
Topicity of Ligands

Welcome back to the course entitled symmetry, stereochemistry and applications. Previous class we have discussed about the topicity of different carbon centers. So we will continue our discussion in this direction today.

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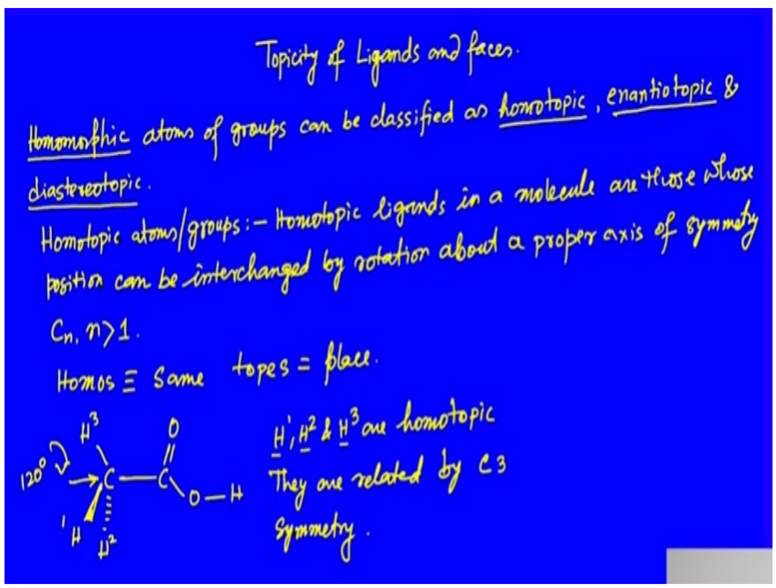

So in today's class we will discuss about topocity of ligands and faces so in a molecule there are different atoms or group of atoms that are connected to different carbon centers. And then when we have similar group of atoms in a molecule what we see is that by replacing of those groups by a different group can result in different types of molecules. So we can say that homomorphic atoms or groups can be classified as homotopic, enantiotopic and diastereotopic.

So homomorphic atoms means the atoms which are same or groups which are same. So now we will try to define these 3 different types of topicities of the ligands or the groups that are associated with a carbon center. So let us start the discussion with homotopic atoms or groups. Homotopic ligands in a molecule are those whose position can be interchanged by rotation about a proper axis of symmetry.

That is Cn with n greater than 1 in Greek homos means same and topes means place so let us try to understand the topocity of different hydrogen atoms that are connected to this carbon atom which is the first carbon atom of acetic acid. These hydrogen atoms which are marked here as 1, 2 and 3 these 3 hydrogen atoms H1, H2 and H3 are homotopic because they are related by C3 symmetry.

So by rotation about this axis 120 degree rotation H1, H2 and H3 can interchange their places without doing any change in molecule. Therefore these 3 hydrogen atoms are can be termed as homotopic hydrogen atoms. Let us try to take another example.

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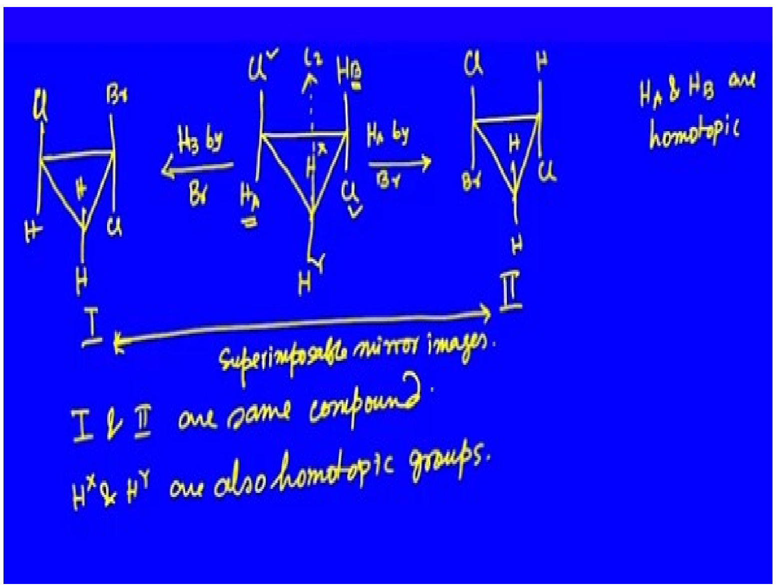

An example of a cyclic compound cyclo propane in which I have 2 chlorine atoms in the trans position. So the hydrogen atoms marked A, and B are homotopic why because this HA and HB can interchange their places. If I rotate the molecule through this C2 axis then this hydrogen will go there and this chlorine will come here and the molecule will remain unchanged. Now there is another way to test whether they are homotopic or not?

So what we are trying to do is now we are trying to replace HA by bromine so what we get is this molecule. And on the other hand if we replace HB by bromine what we get is this molecule suppose these are compound number 1 and 2 originating from the parent compound. So what is the relationship between these 2 compounds 1 and 2 if you look at it carefully they are super imposable mirror images.

Therefore 1 and 2 are same compound right if we look at the other 2 hydrogens HX and HY, the same relationship is valid HX and HY are also homotopic groups.

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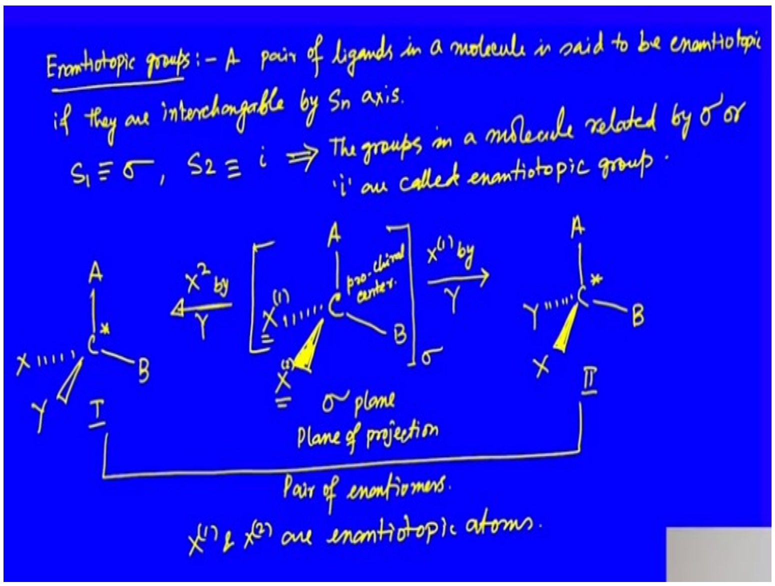

Now let us try understand what happens when we call as group as enantiotopic? A pair of ligands in a molecule in a molecule is said to be enantiotopic if they are interchangeable by Sn axis. And as we know S1 is equivalent to sigma plane and S2 is equivalent to i that means the groups in a molecule related by a sigma or i are called enantiotopic groups. What happens when you substitute those enantiopotic groups by another atom one after another one by one?

You can generate 2 molecules which are essentially enantiomers and from the product that it generates as enantiomers we call that those 2 atoms are pair of atoms as enantiotopic atoms. So let us try to see this with one example, suppose we have a chiral center with 2 different groups A and B and carbon center with 2 groups A and B and 2 atoms which are identical X. These 2 groups are related by a sigma plane that is the plane of the projection.

This plane of projection is your sigma plane and if we replace suppose if I tell this as X 1 and that X as X 2. If we replace X 1 by Y we would get this molecule and if we replace on the other hand X 2 by Y we would get this molecule. This molecule 1 here and this molecule 2 they are pair of enantiomers therefore these atoms X 1 and X 2 are enantiotopic atoms. Hope I am able to make you understand what does enantiotopic groups or enantiotopic atoms mean?

What you can see here is that this particular carbon has become a chiral center after replacement of 1 of the 2 enantiotopic groups. So this chiral center this carbon center is called a pro chiral carbon or pro chiral center. Let us see this with another example.

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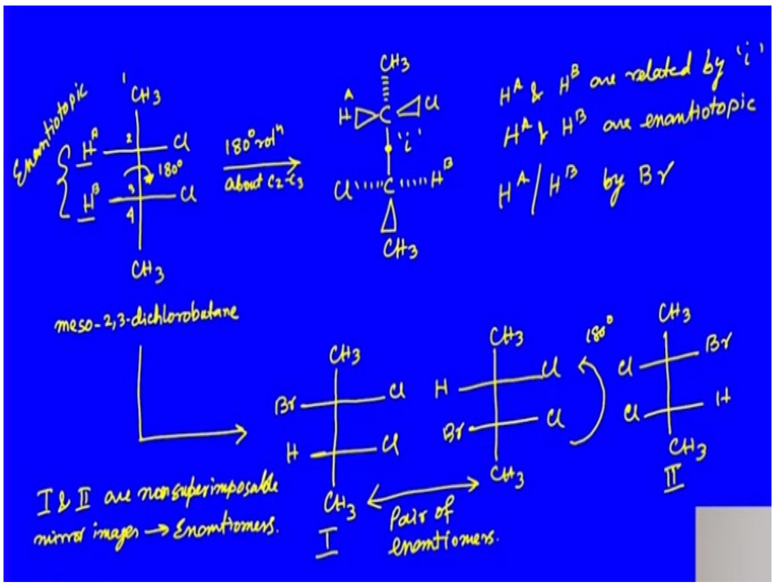

Suppose if we take this molecule, what is the molecule, this is a meso compound. So we write it as meso 2, 3 dichlorobutane, so this compound has 2 hydrogens namely H A and H B. If we rotate about this bond by 180 degree what we would get? We would get this arrangement just by rotating about C2 C3. So what do we see in this molecule? This molecule as an inversion center i and this hydrogens H A and H B are related by the inversion center i.

Therefore HA and HB are enantiotopic let us try to see what happens if you replace H A or H B one after another by bromine. So at first if we replace H A by bromine and leave H B as it is we get this molecule. And if we replace H B by bromine and keep the hydrogen intact, what we get are a pair of enantiomers. How do we see that these are pair of enantiomers? We take this molecule and rotate the entire molecule in plane by 180 degree and we get this orientation.

When you rotate this molecule by 180 degree these 2 chlorines will come to the left hand side this bromine will come here and the hydrogen will come here and this CH3 groups will remain as it is. So now can we see that this group molecule 1 these molecule 2 are mirror image of each other and they are non-super imposable mirror image. So 1 and 2 are non-super imposable mirror images therefore they are enantiomers.

Therefore these 2 hydogens can be termed as enantiotopic hydrogens let us take one more example.

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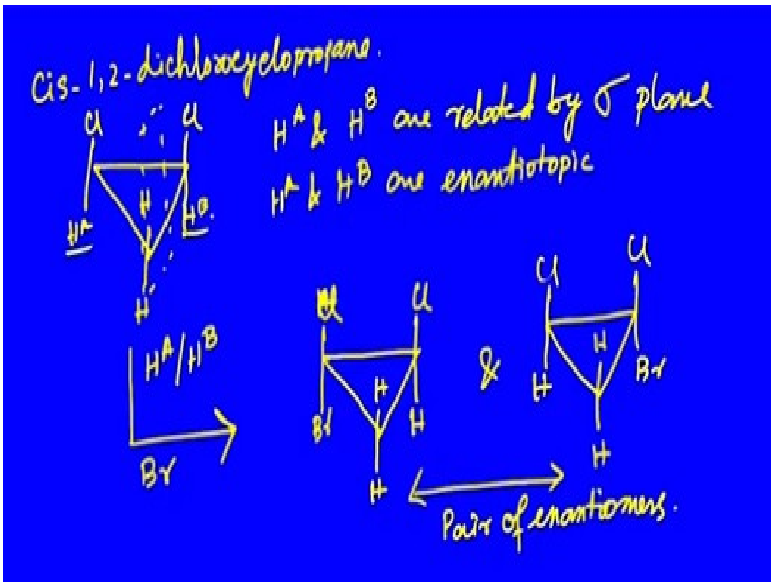

Cis 1, 2 dichlorocyclopropane so in this case let us first draw the molecule this H A and H B are related by a sigma plane that is the plane which bisects the molecule in this perpendicular direction. Therefore H A and H B are enantiotopic. So now if we try to simply replace H A and H B by different group. If we try to replace this H A or H B by a bromine we would generate 2 compounds which I am drawing now.

These 2 compounds are again a pair of enantiomers therefore these 2 hydrogens can be termed as enantiotopic hydrogens.

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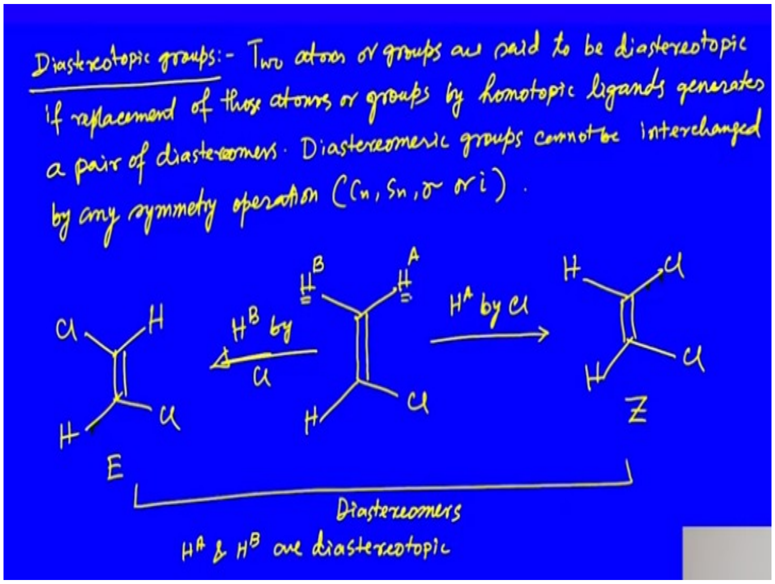

Now let us move to diastereotopic groups, from the name itself you can now understand that by replacement of 2 atoms by different groups it should generate a pair of diastereomers. So the definition is 2 atoms or groups are said to be diastereotopic if replacement of those atoms or groups by homotopic ligands generates a pair of diastereomers. Diastereomeric groups cannot be interchanged by any symmetry operation that is Cn, Sn sigma or i.

Let us try to see this with one example. Let us take the example of this chloro ethene here we have 2 hydrogens H A and H B. If we replace H A by chloro we get this compound and if we replace H B by Cl we get this compound. So this is the z isomer and this is E isomer of the 1, 2 dichloro ethene and these 2 compounds that we have formed we know are diastereomers because they are not mirror image relations.

So these 2 hydrogens H A and H B are distereotopic and you see that there is no symmetry operation that can interchange H A with H B. So let us try to see this with 1 more example of cyclo propane which has 2 substitutions chloro and fluoro.

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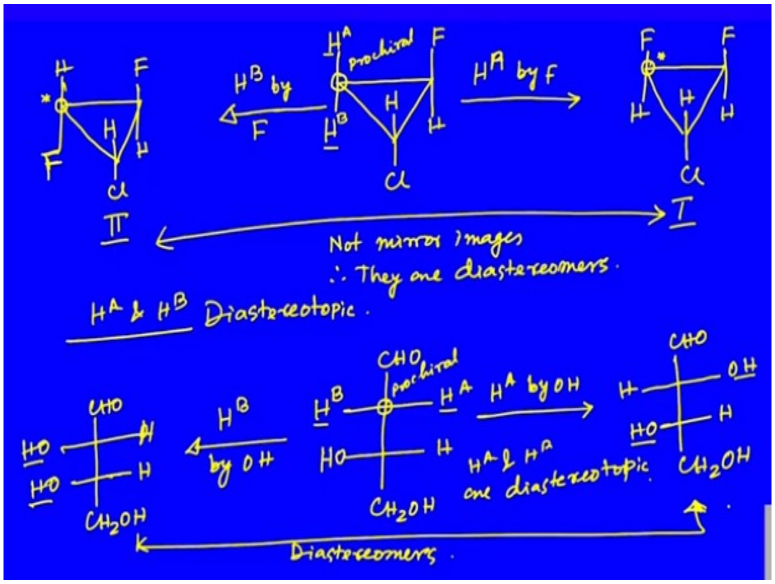

In the trans position. so this H A and H B that I have marked, let us see what happens when you replace H A and H B separately by F. So what we see here is that point 1 this H A and H B cannot be interchanged by any symmetry operation C2 Cn or sigma or i. And then when we replace H A by F we get this molecule when we replace H B by F we get this molecule what we see here is that this F and F are trans here the 2 F's are Cis.

Therefore these 2 compounds are again they are not mirror images, therefore they are diastereomers, a pair of diastereomers. So those 2 hydrogens H A and H B they are diastereotopic. Let us see with one more example how this diastereotopic hydrogens can be easily identified. See in the previous example also this particular center was not chiral center it was a pro chiral center but after replacement of fluorine that center has become a chiral center. Because now you have 4 different groups attached to that.

Similarly here you see that this particular carbon is pro chiral and these 2 hydrogen atoms H A and H B are not related by any symmetry. So now if we replace H A by O H, I am sorry here this should be OH. And if we replace on the other side H B by O H what we get is this molecule. What we notice here is that in this molecule you have both the OH groups on one side here the 2 OH groups on the opposite side.

So these 2 compounds are diastereomers so this H A and H B are diastereotopic. So we conclude this lecture today with a note that today we have discussed about homotopic enantiotopic and diastereotopic ligands. So in the next lecture we will discuss about the homotopic, diastereotopic and enantiotopic faces of molecules.