Symmetry, Stereochemistry and Applications
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Module No # 05
Lecture No # 24
Topicity of Faces

Welcome back to the course entitled symmetric stereochemistry and applications. We will continue from the previous lectures when we were discussing about topicity of various ligands. So in this lecture we will talk about the topicity of faces.

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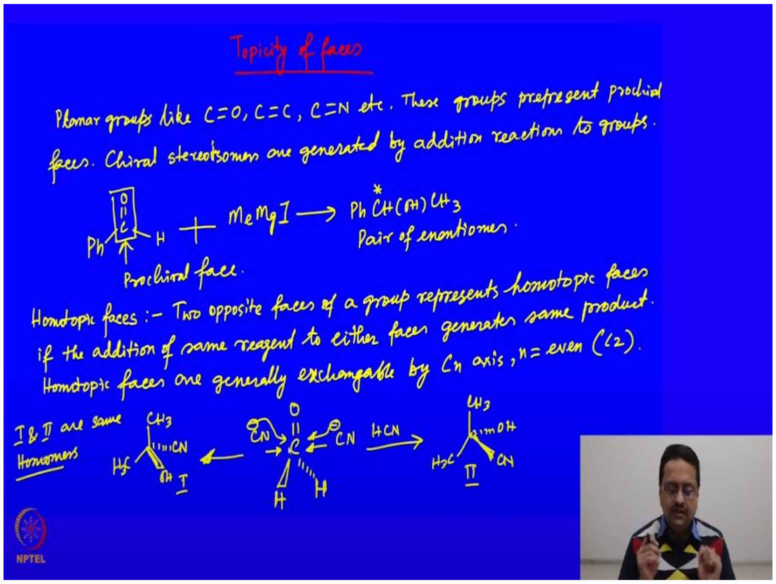

Topicity of faces

Planar groups like C=O, C=C, C=N etc. These groups prepresent prochiral faces. Chiral stereoisomers are generated by addition reactions to groups.

$Ph-C(=O)-H + MeMgI \longrightarrow Ph\overset{*}{C}H(OH)CH_3$

Pair of enantiomers.

Prochiral face.

Homotopic faces :- Two opposite faces of a group represents homotopic faces if the addition of same reagent to either faces generates same product. Homotopic faces are generally exchangable by C_n axis, n = even (C_2).

I & II are same Homomers

So in organic molecules we get many planar groups like C double bond O, C double bond C, C double bond N etc., And these groups represent pro chiral faces and what we see is that chiral stereoisomers are generated by addition reactions to these groups. So for example if we have PhCOH and we add methyl magnesium iodide to that and then do the corresponding hydrolysis we get PhCHOHCH3 and we generate a chiral center in this molecule and we generate it as a pair of enantiomers.

Therefore we call this groups or this as a prochiral face. If the reaction takes place from the top this group or from the bottom of the group it generates 2 different stereo isomers. So, as just like the different groups which we homotopic, enantiotopic and the diastereotopic group. Here also faces can be identified as homotopic, enantiotopic and the diastereotopic. So let us try to first understand what are homotopic faces?

2 opposite faces of a group represents homotopic faces if the addition of same reagent to either faces generates same product. Homotopic faces are generally exchangeable by Cn axis where n is even, say C2. So if I draw this molecule which his nothing but formaldehyde by now you have learnt what does this representation mean? Here this C double bond O is in the plane of projection and the H atoms are above and below the plane of presentation.

So we have 2 faces one is from this side and one is from the other side. So this formaldehyde if we do an addition reaction by cyanide group from the side of the face we would get the product that is I am adding HCN the product would be this one. And if we do the reaction from the other side we would get these as the product. On careful look at this 2 product you can easily identify that these 2 compounds are same compounds.

So one this product 1 and 2 are same that is they are homomers. Therefore in this molecule, formaldehyde, the faces of formaldehyde are homotopic faces. Let us try to see another example.

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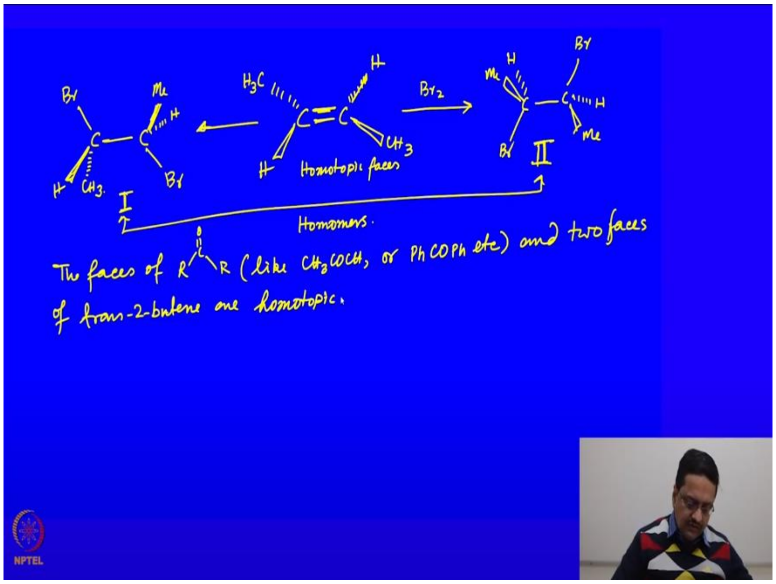

The faces of $R\overset{O}{\overset{\|}{C}}R$ (like CH_3COCH_3 or PhCOPh etc) and two faces of trans-2-butene are homotopic.

Let us take the case of trans 2 butene and if we do addition of bromine to this molecule this reaction happens through the formation of bromonium ion and we would get the addition product as this one or we would get the addition product as this one. So these 2 compounds are one and the same. Therefore the 2 faces of this C-C double bond are homotopic faces. I leave it to you to draw the Fischer projection of these 2 molecules and identify that these 2 molecules are one and the same.

Similarly the faces of R C double bond O R like CH3COCH3 or benzophenone that is PhCOPh etc., and 2 faces of trans 2 butene are homotopic. Now let us see how do, we can identify the enantiotopic faces.

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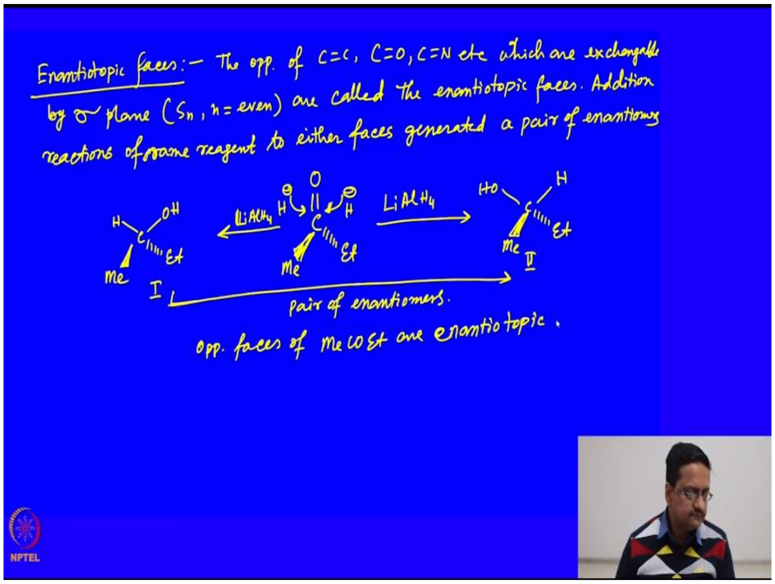

Enantiotopic faces:- The opp. of C=C, C=O, C=N etc which are exchangeable by σ plane (S_n, n = even) are called the enantiotopic faces. Addition reactions of same reagent to either faces generated a pair of enantiomers

opp. faces of MeCOEt are enantiotopic.

The opposite faces of C double bond C, C double bond O, C double bond N etc., which are exchangeable by sigma plane that is Sn with n equal to even, are called the enantiotopic faces. Addition reactions of same reagent to either faces generates a pair of enantiomers. So let us see with 1 example, we take the example of a ketone with 2 different groups attached to it. So if we add hydride from the right hand side using lithium aluminum hydride reagent, our product would be this one.

If we do the same reaction from the opposite direction that is reduction by lithium aluminum hydride we would get the opposite product. So here these 2 compounds 1 and 2 if you look at them carefully you will see that they are pair of enantiomers. Therefore these 2 faces the left hand side face and the right hand side face of this molecule are enantiotopic. So the opposite faces of MeCOEt are enantiotopic.

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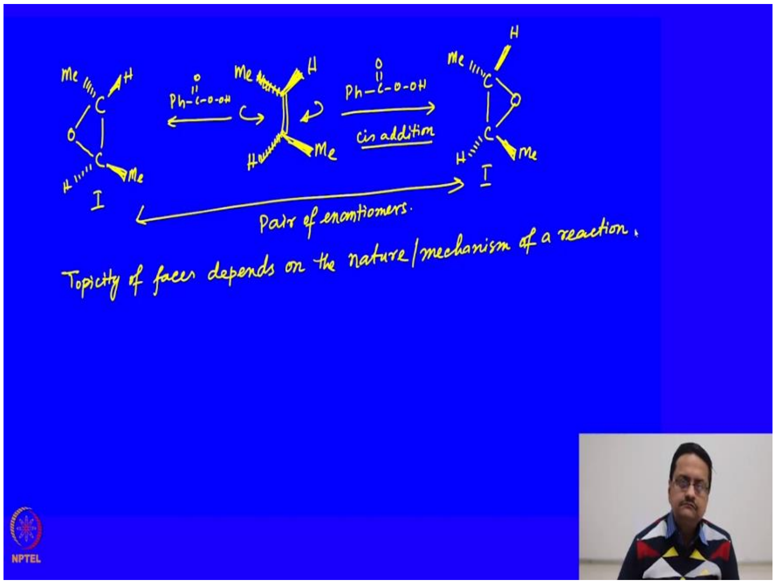

Pair of enantiomers.

Topicity of faces depends on the nature/mechanism of a reaction.

Let us take one more example let us take the case once again of trans 2 butene. If we do the addition of per oxy benzoic acid from the right hand side we would get, let us draw this in the form of wedge and dash projection for your easy understanding. So the product that we would get is this one. The epoxide will form in such a way that we will get a pair of enantiomers. These 2 compounds, 1 and 2 are pair of enantiomers.

Therefore what we can see here in case of 2 butene when we had done the reaction little while ago using a bromine addition which I did not mention at that time is a trans addition reaction, you will see the mechanism of this reaction in a later lecture. This bromine addition being a trans addition reaction these 2 faces are homotopic faces. But when, we see this reaction which is a Cis addition.

Therefore the same pair of faces now turns out to be enantiotopic faces. So one can say that topicity of faces depends on the nature or mechanism of a reaction. Now let us try to define the diastereotopic faces.

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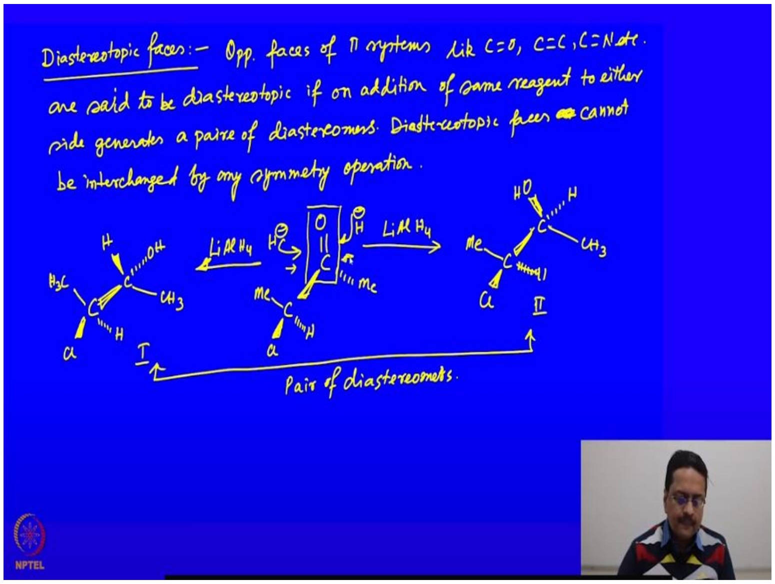

Diastereotopic faces:- Opp. faces of π systems lik $C=O$, $C=C$, $C=N$ etc. are said to be diastereotopic if on addition of same reagent to either side generates a paire of diastereomers. Diastereotopic faces cannot be interchanged by any symmetry operation.

Opposite faces of Pi system like C double bond O, C double bond C, C double bond N etc., are said to be diastereotopic if on addition of same reagent to either side generates a pair of diastereomers. Remember that diastereotopic faces cannot be interchanged by any symmetry operation. So let us try to see this with one example. Suppose we take a molecule which already has a chiral center.

For this molecule we are trying to understand the topicity of faces carbonyl group. So what we are trying to do is to do the same lithium aluminum hydride reduction assuming that hydride comes from the right hand side. So in that case the product, supposed to be this one. But if we do the reaction of reduction from the right hand side by lithium aluminum hydride what we get is this product.

These 2 compounds, 1 and 2 you can easily understand that they are a pair of diastereomers. Please try to draw the Fischer projection of these 2 compounds yourself and see that these 2 are diastereomers. So these 2 faces that we are trying to talk about are diastereomeric faces.

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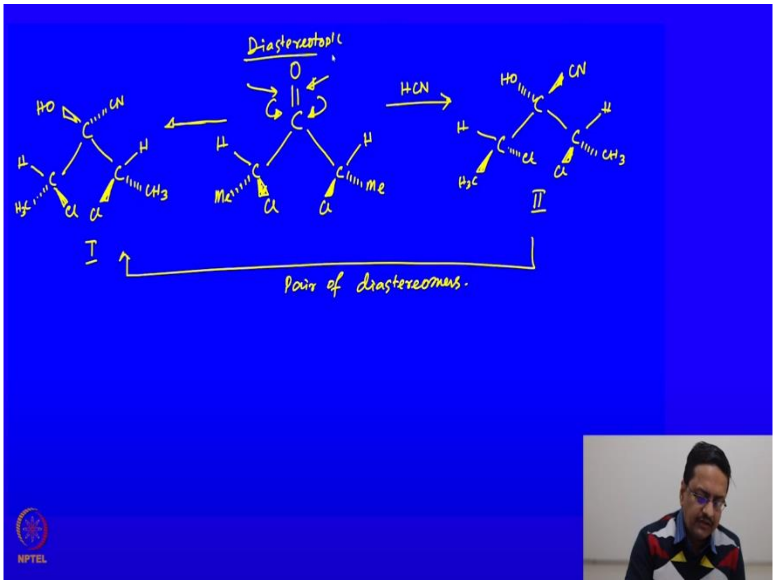

We take another example here and if we try to add HCN to this molecule from this side and from the other side what we would get are these 2 compounds. Here this compound 1 and this compound 2 once again are pair of diastereomers. Therefore these 2 faces which we are talking about are diastereotopic faces. So we can summarize what we have learnt in last couple of lectures. What we can do is?

We can classify these different groups and faces in 3 different classes like homotopic, enantiotopic and diastereotopic. So we can easily draw a table and summarize these 2 lectures. The headings of the table are the following.

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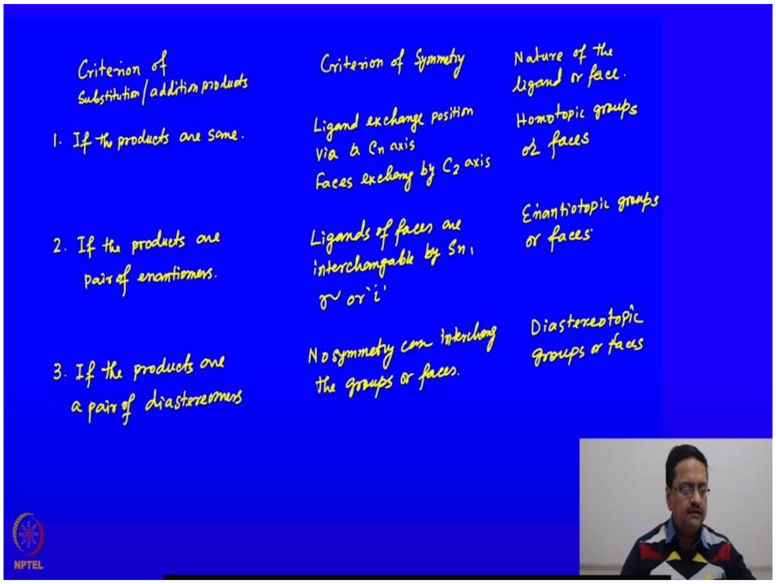

Criterion of Substitution/addition products	Criterion of Symmetry	Nature of the ligand or face.
1. If the products are same.	Ligand exchange position via a C_n axis Faces exchang by C_2 axis	Homotopic groups or faces
2. If the products are pair of enantiomers.	Ligands of faces are interchangable by S_n, σ or 'i'	Enantiotopic groups or faces
3. If the products are a pair of diastereomers	No symmetry can interchang the groups or faces.	Diastereotopic groups or faces

Criteria of substitution or addition products, criteria of symmetry and the nature of the ligand or face, so the first point is if the products are same then the ligands exchange position via the Cn axis or the faces exchange by C2 axis then those groups or faces are to be termed as homotopic. Condition number 2, if the products of substitution or addition reactions are a pair of enantiomers then the ligands or faces are interchangeable by Sn, sigma or i.

Then those groups are called enantiotopic groups or enantiotopic faces. The third one is if the products are a pair of diastereomers. Then no symmetry can interchange the groups or faces. They are called the diastereotopic groups or faces. In this context I would like to introduce you to another method of nomenclature of these different groups and faces or rather the faces.

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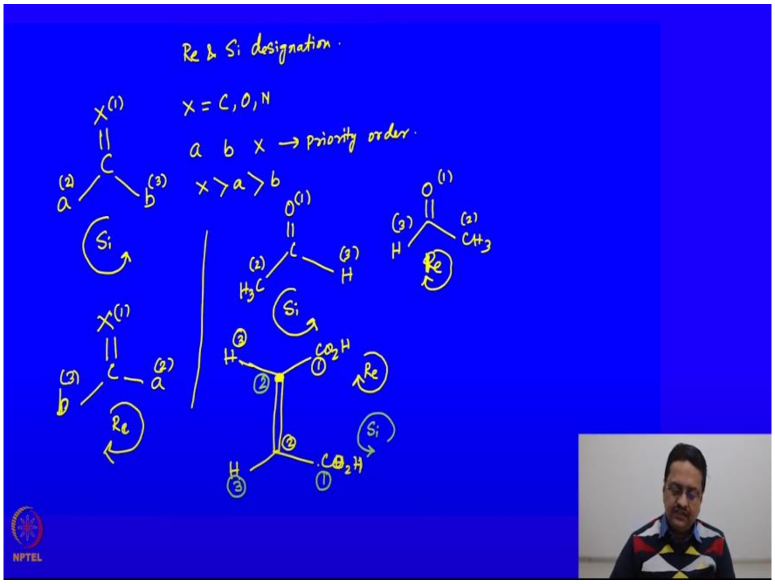

Re & Si designation.

$X = C, O, N$

a b X → priority order.

$X > a > b$

So this is called the Re and Si designations. So suppose we are trying to talk about a group C double bond X is connected to 2 different groups a and b where X can carbon, oxygen and nitrogen. So when we see this group we first try to identify these groups a, b and x in terms of their priority order. Suppose if x has higher priority over a, and a has higher priority over b then this X is given priority 1 and a is given priority 2 and b is given priority 3.

So now if we do go from 1 to 2 to 3 we are going in anticlockwise direction. So this particular face which is from the top of this molecule is designated as the Si face and if we draw the molecule in such a way that the opposite face is facing us that is a here and b there and then 1 to

2 to 3 is in clockwise direction just like R. So this face is called the Re face. So let us try to see this with a couple of real examples.

Suppose if I look at this molecule, here oxygen having the higher atomic number gets priority 1, carbon here gets priority 2 and hydrogen gets priority 3. So this particular face of this molecule is looked as 1 to 2 to 3 in anticlockwise direction. So, it is a Si phase and the other face which is below face can be drawn like this again priority 1, 2 and 3. It is 1 to 2 to 3 is clockwise direction. So this is the Re face.

If we take the example of a C- C double bond maybe having 2 carboxylic acid groups in the Cis orientation what we see here now the priorities are changed. Here carbon gets priority 1 because carbon is then connected to oxygen. This carbon is connected to another carbon so gets priority 2 and this hydrogen gets priority 3. So for this particular carbon this face is 1 to 2 to 3 is Re. For the other end this carbon gets priority 1, this gets priority 2, this gets priority 3.

So here this is 1 to 2 to 3 is anticlockwise direction. So it is the Si face. So I would like you to see this from a standard text book and go through further examples and learn it yourself. So we can conclude this lecture at this point and we will continue from here in the next class.