Course on Stereochemistry
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Module No 03
Lecture 10: Topicity

Okay so in the last lecture we have seen what are the ways to determine the absolute configuration of the molecule or the nomenclature systems that are used to describe the absolute configuration and to describe the relative configuration okay? Now in this lecture, we will now bring in another topic which is the which is basically based on the relationship between the ligands that are present in a molecule, the ligands that are present in a molecule, the ligands that are present in a molecule, the relationship between the ligands.

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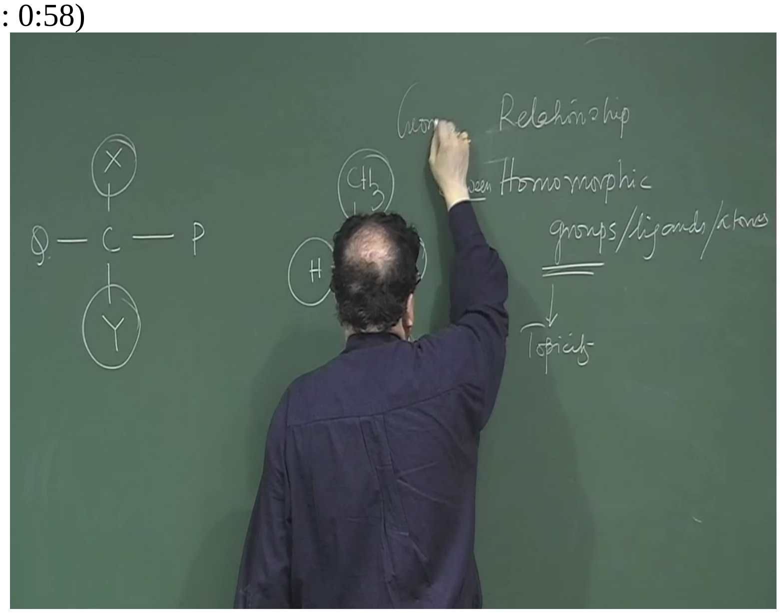

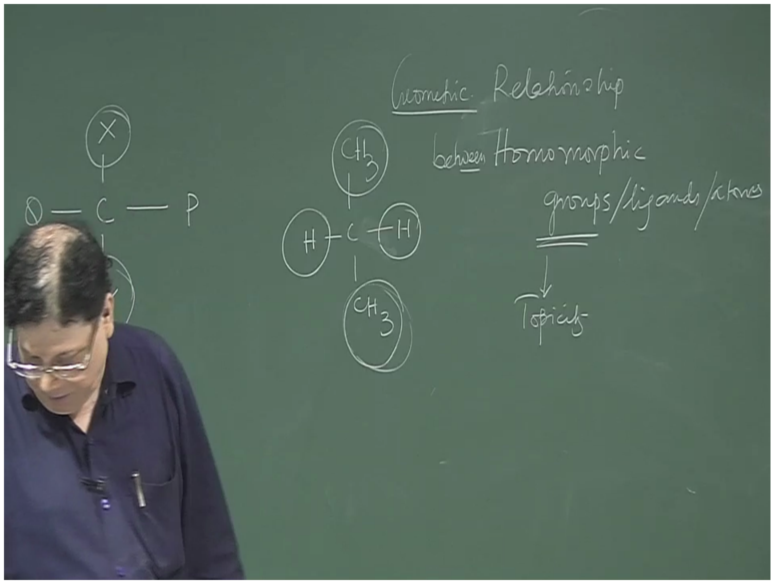

Like if you have a carbon and if I have 2 ligands attached to this carbon, of course it has to attach to 4 ligands, say XY, say P and Q and and if I want to know their relationship between this text and why, earlier what we have done, we have done the, the absolute configuration of these. We always concentrated on the stereogenic Centre. Now in a departure from that, what we are doing now?

We try to see that what is the relationship between the ligands that are present in a in a molecule in a three-dimensional molecule which can exhibit stereochemical attributes okay? So this little bit different. We are not talking about the stereogenic centres. We are talking about the ligands, what is the relationship between the ligands in a molecule okay? Now this X, Y, P, we remove this, we put some groups.

Suppose we put a methyl, we take this very simple compound, C H2 and CH 3 okay? The the pentane. Now in this pentane sorry propane at the carbon, this carbon has these 2 hydrogens and if I want to know the relationship between these 2 hydrogens, now if I, if I want to look separately, not from the molecule, if I segregate this hydrogen, take this ligand out of this carbon and take this ligand out of this carbon.

They are same motherboards are hydrogens or take this methyl, just look in isolation, okay this is methyl and look in isolation of this group. This is also methyl. So these 2 groups are same. These are called isomorphic these are called sorry homo homomorphic groups sorry homomorphic groups. Homomorphic groups means groups which are in isolation look the same. They look the same means they have the same Constitution.

Then they are called homomorphic groups or homomorphic ligands. Like these two methyls, they are homomorphic ligands. Like the 2 hydrogens, they are homomorphic ligands. Now we want to know the relationship between these ligands and this relationship is what is called topicity. So relationship between homomorphic ligands between homomorphic groups or ligands or atoms, whatever it could be just atoms. That is what is called topicity. What type of relationship? Geometric relationship or you can say stereochemical relationship between the homomorphic groups or ligands or atoms okay?

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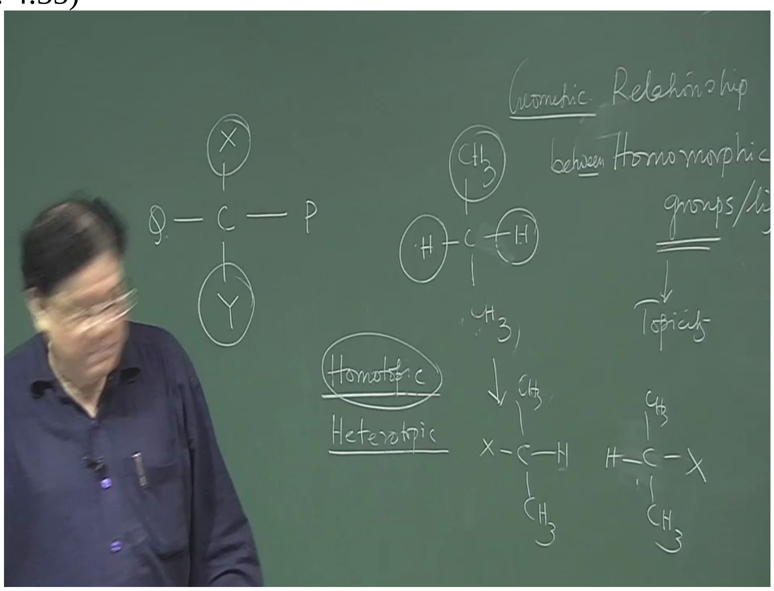

Now there are different types of relationships that is possible. One is called, I said this relationship is called topicity. So whatever the name given to these ligands, set of ligands will be will have something in front before topic okay? Like Homotopic, there are set of ligands which are Homotopic. There are set of ligands which are heterotopic okay? Homotopic or heterotopic. Now the name suggests that Homotopic means like homomers I had said earlier, same molecule.

So Homotopic means, there is no difference between the groups for the ligands or the atoms that we are considering okay? 1st of all, they have to be homomorphic, that means they have to be same. Otherwise there is, the comparison, you cannot compare chlorine with fluorine. They are different ligands. So we are comparing either 2 chlorines or 2 methyls or 2 hydrogens or 2 fluorines but out of that, you can have various situations where both the suppose these 2 hydrogens if I consider, these 2 hydrogens can be Homotopic or heterotopic depending on the structure of the molecule okay?

Now structure of the molecule and the way to determine whether they are topic or heterotopic, heterotopic means they are now starting to deviate, they differentiate, they can be differentiated okay? How to do that? There are there are 2 ways. You can consider symmetry elements to decide the topicity of ligands or you can consider what is called substitution addition criteria. The substitution addition criteria is the more appealing one, the easier one okay?

So what it says? That if you want to know what is the what is the relationship between these 2 hydrogens, so you replace one of the hydrogens with a group X and then keep the molecule in the the other groups area okay? So you get this compound. On the other hand, if you replace the other hydrogen with X, so you get the, you get this compound. Now you are asked, what is the relationship between these 2 compounds?

Are they saying? Are they stereoisomers or are they constitutional isomers or whatever. So try to find the relationship between these 2. Now they are actually same because there is 1st of all, their constitution is same and there is no question of stereoisomerism here because there is no stereogenic Centre because this is attached to 2 methyls, same ligand. To have stereoisomerism, we should have stereogenic Centre.

Interchange of groups does not lead to any stereoisomer. So they are same. So if they are same, then that will be called Homotopic. I think it is clear. That will be called Homotopic. In symmetry terms, to find the Homotopic, we have to find whether there is a C axis present here or not okay? Like this molecule has a C2 axis. Like if you put an axis like this and then rotated by 180, this hydrogen will be there, that hydrogen comes here, methyl goes there down, this methyl goes up but it remains the same.

So it has got a C axis. That means, the proper axis, the proper element of symmetry, if that is present, then also you can say that they are Homotopic. So you can do 2 things, either you do this this replacement of groups, that means, that is called substitution addition method or you can check whether what type of symmetry elements this process. If it possess a C2, then this these 2 ligands are Homotopic okay?

Similarly, you can say that these 2 methyls are also Homotopic. You can do the same substitution addition thing and you can arrive at the same configuration okay between the 2 methyls. Now this is Homotopic. How do we arrive at heterotopic, heterotopic ligands?

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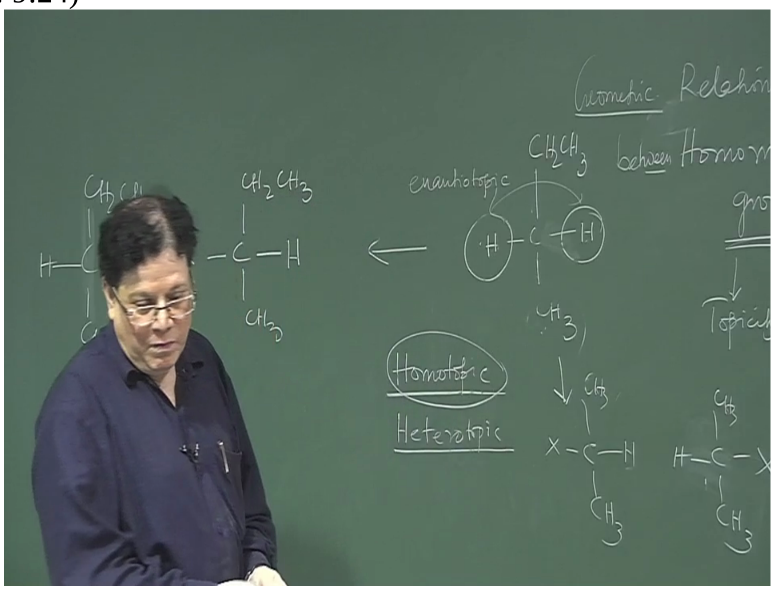

Suppose I put a here CH 2 CH 3, so this is now I just increased the carbon by 1. So CH 3, then CH 2, then CH 2, then CH 3. And I asked, what is the relationship between these 2 hydrogens? Okay? So what you do? You again do the same substitution addition criteria. So I substitute the left hydrogen by X. I get this, I substitute now the right hydrogen by X. So I will get this, CH 2 CH 3 and this is CH 3. Now find out the relationship between these 2.

So what is the relationship between these 2? You can tell they are mirror images of each other. They are enantiomers now okay? So these 2 hydrogens are not the same now. Earlier, in Homotopic system, they are leading to the same compound. Here, there is a difference. So this difference tells you difference means they are now leading to enantiomers, not only stereoisomers but enantiomers.

So these 2 hydrogens will be called not only heterotopic but they will be called enantiomers. They will be called enantiotopic okay? And there is see it is not necessary always that you consider the ligands attached to the same carbon.

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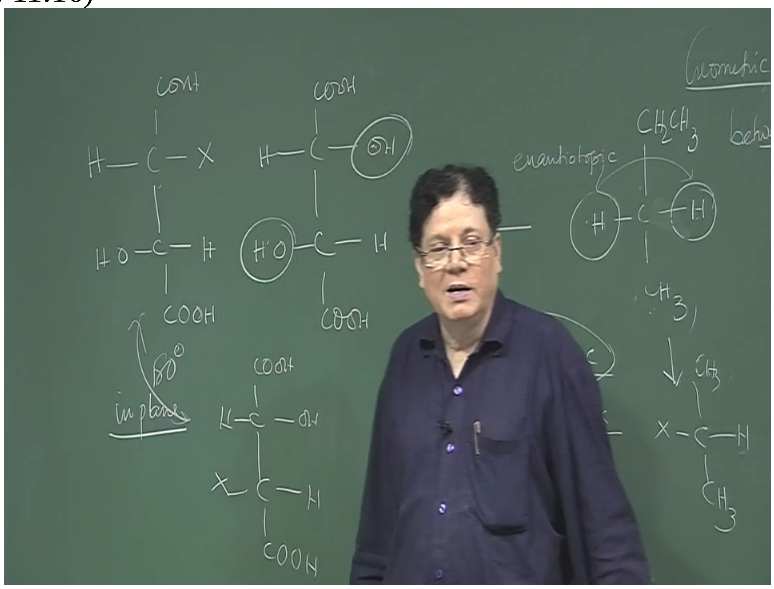

You can you can also do it for different carbon. Suppose if I ask that what is the relationship between these 2 hydroxy groups, they are homomorphic ligands because they are both OH, constitutional they are same. So what is the relationship between these 2 OHes? So how do you do? Again, apply the addition, that principle substitution addition principle. So you put X there, CO2H and CH keep the other one intact okay?

So you get this compound. And you replace this one, the bottom one, if you do that, what you end up is OH, H, C, X and COOH. Now what is the relationship between this and that? What is the relationship between this and that? You can, you know that Fisher projection formula can be rotated in plain by 180 degree. That is allowed. So to know the relationship between this and that, what you do?

You rotate this by 180 degree in plain and if you do that 180 degree in plain rotation, in plain rotation, you see this is going to that one or that is coming to this one. That means they are same. So what is the relationship between these 2? Now? So they are Homotopic because the definition of Homotopic is that the substitution is the substitution addition gives the same compound okay? They are giving the same compound. So these 2 0Hes are Homotopic.

Now if you consider that the earlier another concept, the symmetry concept I said if there is a C2, then that becomes Homotopic and you see, there is a C2 here. If you rotate it by 180, it comes to the same molecule, it becomes, it remains the same molecule. So it has got a C2. So these are Homotopic ligands. So that is the way to do.

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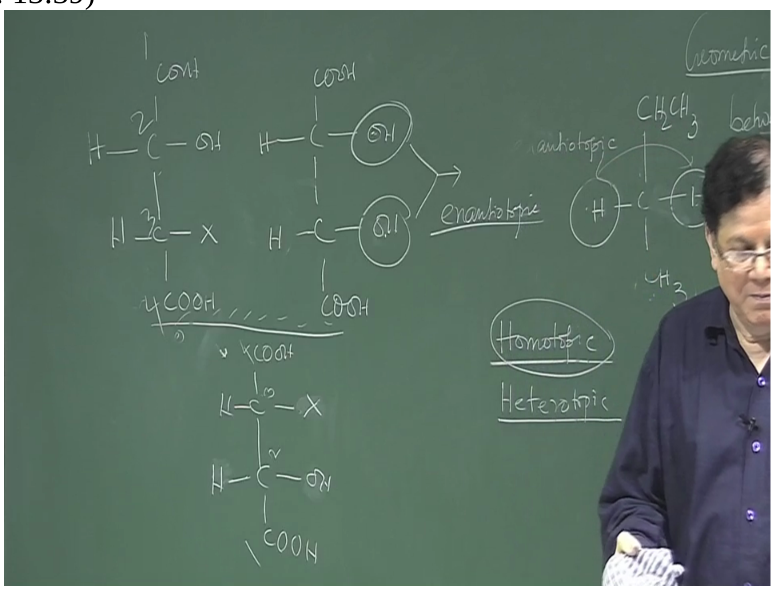

Interestingly if you replace this, change the position of the OH this side, then if I ask what is the topicity of these 2 hydroxy, you see you again do that replacement 1 but now you have 2 OHes on the right. So you replace the top one by X, the bottom one remains and here you replace the bottom one by X, the top one remains there okay? Now you check what is the relationship between these 2.

Now you cannot actually interconvert them. See if you rotate it by 180 degree it X and OH goes to the left side but here X and OH are always on the right side. So what is the relationship between these 2? If you put a mirror here now, so this carbon goes to the top carbon, so that becomes top except best is put the numbering system, 1, 2, 3, 4. So this will be your 4, that will be your 3, that will be your 2, that will be your 1 okay?

So they are just mirror images of each other. So you get mirror image systems by this addition by the substitution addition principle. So these 2 OHes are then, they are enantiotopic okay? And in terms of symmetry elements, I gave you how to go Homotopic, Homotopic ligands are connected by C2, heterotopic ligands, if they are enantiotopic then they are connected by either Sigma like here you see there is a Sigma plane.

Here there was, earlier there was C2. So that made the 2 OHes Homotopic. Now these OHes are on the same side. So C2 is gone now but in what is there now is a plane of symmetry. Those are called improper elements of symmetry. So when there are improper elements of symmetry present, the ligands become enantiotopic okay? Improper elements of symmetry means it could be I, it could be Sigma or it could be S okay?

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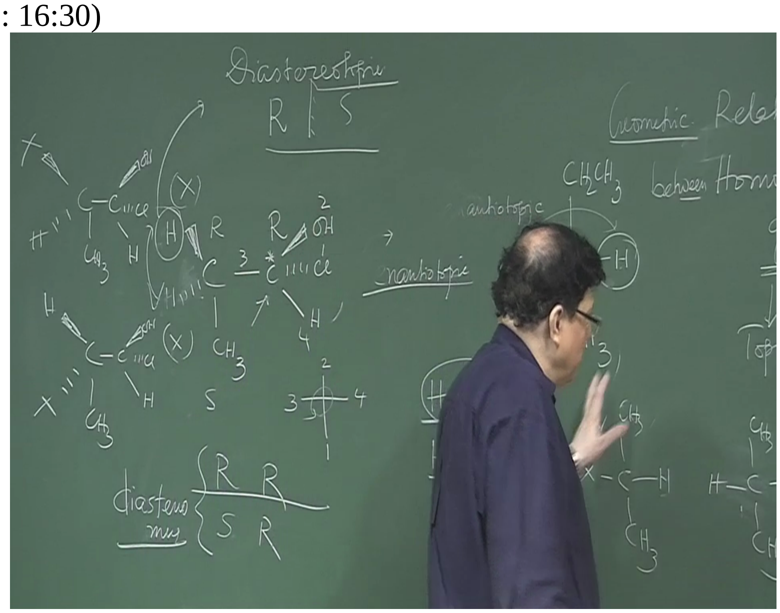

And finally there is one more topicity which one should know and that is again I bring very similar molecules stereo topic sorry, not this one. I make, I create a molecule, now I actually take the advantage of the OH formula. Suppose this is OH, this is CL and this is H, and then I have a CH 2 here and a CH 3. So I consider this molecule. That means I have a molecule which already has a breach in chirality here as stereogenic Centre with a particular configuration.

What is the configuration? You can determine this is your one, that is your 2, that is your 3 and then you have to check what is the hydrogen, the 4th group and you can assign the configuration.

But I started with a compound with a particular stereochemistry here okay? And then I am asking, what is the relationship between these 2 hydrogens? Okay? Let us try to do the RS configuration if you want.

If you try to do the RS configuration, this is suppose see I draw the Fisher projection, this is 1, that is 2, this is 3, this is 4. So in the Fisher Fisher position, I should look through the bonds which are similar. So I look from this site. So this is 4, this is 3, this is 2 and that is 1. 4 is on the horizontal side. So whatever I see, it should be the other way around. So 1, 2, 3 it appears to be clockwise anticlockwise.

So that should be R configuration. So you have R configuration here. Now what is the relationship between these 2? Now among these 2 hydrogens, see one will be beta, another will be alpha okay? So if you if you replace this hydrogen by X okay, by X or it and then put the hydrogen here, keep the hydrogen here and replace this by X. So either replace this by X or replace this by X. What will be the relationship between the 2 molecules?

Now to know that, one basic principle, one should learn and that is the image of R is S okay? So when you put a group X here, this becomes a stereogenic Centre. So it will have a configuration. When I put X here, that will also have a configuration. Suppose by replacing this hydrogen with X, this becomes R, and suppose replacing this hydrogen by X, this becomes S, so basically what I am getting is a RR compound because this R was already there built in.

And here, I am getting SR. So what is the what will be the relationship between the 2 molecules that I will be generating? See I can draw this. So that will be X, that will be hydrogen, that will be methyl and this remains the same, OH, CL, H. And the other molecule will look like X, then this is hydrogen, this is methyl and this is C, it remains the same. What is the relationship between these 2?

These 2 are now no longer enantiomers because I said, R, mirror image of R is S. So the mirror image of RR should be SS. But here, RR and SR, so they are now Diastereomers because enantiomers will be RR or SS or SS or RR. So here, substitution elimination is leading substitution addition sorry I keep on saying elimination, substitution addition creates two Diastereomers.

So these 2 hydrogens then will be diastereotopic will be diastereotopic okay? So basically we have learnt topicity is again to summarise, topicity is basically the relationship, the geometric relationship between the between the 2 homomorphic ligands in a molecule. There can be different types of topicity, Homotopic. Homotopic systems are are connected by C2 axis, number 1.

And substitution addition gives the same molecule in Homotopic system. In enantiotopic system, the ligands are interconnected by either I or Sigma or S. That means an improper element of symmetry is present and by substitution addition you end up creating an enantiomeric pair okay? So that becomes enantiotopic and there is a 3rd scenario where already a stereogenic centre with a particular configuration is already present.

Then if you are trying to compare to homomorphic ligands, you will see that you end up with Diastereomers. So this ligand becomes diastereotopic. And in terms of symmetry, because this is chiral molecule because you have already a built-in chiral centre, so there is no question of any element of symmetry present in it. So basically now we have 3 scenarios. When C2 is present, ligands become Homotopic.

When Sigma, I or S present, the ligands become enantiotopic, when nothing is present, that means the molecule is chiral, then the homomorphic ligands become diastereotopic. What is the utility of knowing this topicity? The utilities that their behaviour towards different reagents okay? Homotopic ligands behave the same to every reagent whether the reagent is chiral or achiral.

Enantiotopic ligands behave similarly towards achiral reagents, that means reagents which do not have any chirality. And heterotop and then diastereotopic ligands behave differently all the time whether it is a chiral reagent or an achiral reagent. There is a spectroscopy called NMR spectroscopy by which you can different state between these ligands okay. Diastereotopic ligands always differ in their the signal whether it comes okay?

Enantiotopic unless you add a chiral solvent, they appear in the same region region okay? And Homotopic ligands always come in the same region, same signal whether it is achiral solvent or a chiral solvent. I hope that is clear. So this is what is the topicity. So we have now done up to the topicity. Next what is remaining is how to assign the absolute configuration of these ligands because these ligands also can be to to know that which hydrogen I am talking about in a system, I have to assign a configuration which are called pro systems, pro R or pro S systems but that we will discuss in the next class thank you.