Symmetry, Stereochemistry and Applications
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Module No # 05
Lecture No # 25
Problems on Isomers and Topicity

Welcome back to the course entitled symmetry, stereochemistry and applications. In the last couple of lectures we have discussed about topicity of ligands and faces. We have discussed about how to identify the distereomers in allene systems and how to identify them as in terms of R and S isomers? So in today's lecture we will discuss about some of the problems that may be asked in the exams that you will face in this course.

Let us understand the subject in depth by solving some of the problems. So I am giving you the example of allene where allene may contain stereo centers as well.

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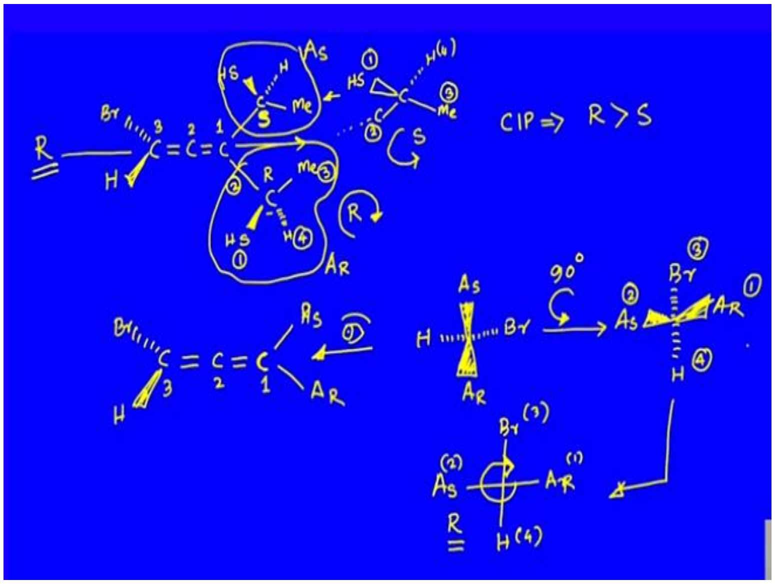

So the question is I am drawing one allene here which in term has a chiral center here with groups as I am marking them H S or S H in the back side one is hydrogen and this one is methyl. Similarly this group has one thiol here back side is hydrogen and this one is methyl. And you have bromine and hydrogen on the other carbon so now if I ask you to identify whether this molecule is R or S we need to first identify the chirality of those 2 chiral centers.

Because otherwise those 2 groups which are there on carbon 1 are identical, the chemical formula is identical. So we will try to name this molecule or identify the chirality of this molecule you first need to identify the chirality of those 2 carbons. So now if we look at the top carbon here what we have is hydrogen at the back which is the fourth priority group highest priority group is above the plane.

And the other 2 groups are here. so in terms of priority this is 1 this groups get priority 2 because this is then connected to carbon another carbon another carbon here another carbon. So this group has overall much larger molecular weight so this is 2 this is 3 so here what we see is 1 to 2 to 3 is anticlockwise. And we are looking from the side opposite to the lowest prior group hydrogen so this must be S. In the same way here this has priority 1 this back groups as priority 2 this has a priority 3 and the hydrogen has priority 4.

So for this carbon if we go from 1 to 2 to 3 we see that it is clockwise so it must be R. So the absolute configuration of this center is R and that top center is S. So now we need to know whether R or S gets priority when they are compared among themselves see according CIP nomenclature rule R gets priority over S. Now let us assume the name of this group as A, so the group with S configuration is AS and the group with R configuration is AR.

So if you draw the molecule now without drawing the large groups as it is we write as AS and AR and draw the other 2 atoms on the carbon 3 as above and below the plane. So now if we are looking at the molecule from this side, as you know does not matter from which side we look at a molecule the absolute configuration does not change. So when we look at this from this side we give priority 1, 2, 3.

And when we were looking at it this carbon 1 has the AS group pointing upwards AR group also pointing upwards. On the back carbon the bromine is pointing downwards on the right hand side and the hydrogen on the left hand side once again pointing downwards. Now this is not the correct way of Fischer projection so what we should do is we should rotate the molecule in plane by 90 degree.

May be in the opposite direction so that the hydrogen which is the lowest priority group comes at the bottom so you rotate it 90 degree in this direction. So what we get is this one so now based on the priorities you know that AR has higher priority over AS, so this is 1 that is 2 this is 3 and hydrogen is 4. Okay anyway let us draw the Fischer projection then we will write the designation.

AR with priority 1, AS with priority 2, bromine with priority 3 and hydrogen with priority 4 so here 1 to 2 to 3 is clockwise. So the absolute configuration is R so the absolute configuration of this chiral axis is found to be R is it clear? So if it is like that then I would like you to try to understand or try to find out the stereo chemical designation of a spiro compound which contains oxygen in the ring.

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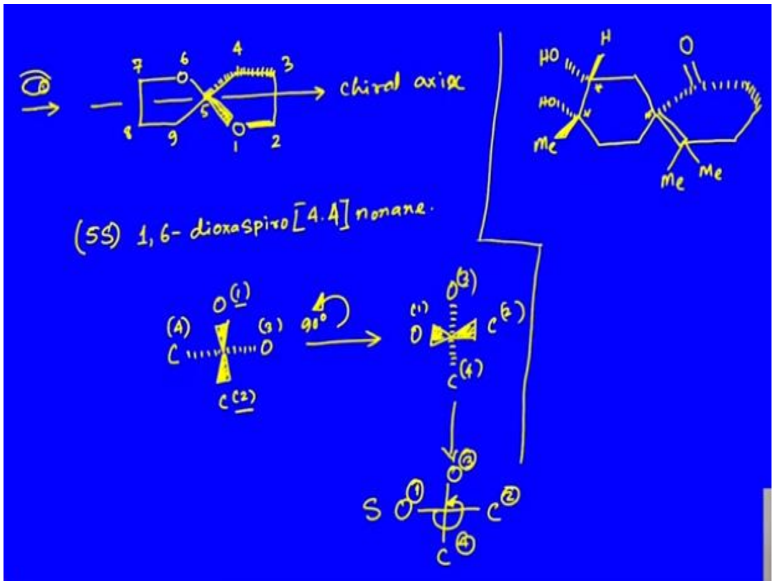

So now you see that this pivot atom at the point from there we should start and number the rings keeping this center untouched. The numbering should be 1, 2, 3, 4, 5, 6, 7, 8 and 9 as per IUPAC nomenclature we should simply write the name as 1, 6 dioxaspiro [4.4] 1, 2, 3, 4, 5, 6, 7, 8, 9. So it is nonane but you see that this compound is now chiral because of that spiro carbon and this being a chiral axis just like a biphenyl system.

So this chiral center as to be identified with the corresponding designation of R or S so now if we look at this molecule suppose from this side what we see is that on the top you have O and bottom you have carbon that those are coming above and below and they are connected. And from his on the right we have oxygen and left we have carbon, which are also connected in turn. So on the first carbon you have priority on this as one this one is 2 this is 3 that is 4.

Now this is not the Fischer projection method because these 2 groups on the carbon 1 are above the plane. So we should rotate it in plane by 90 degree to arrive at this configuration this orientation. Where O1, C2 are like that and O3 and C4 comes like this so if you draw the Fischer projection it should look like this, priorities are 1, 2, 3 and 4. So now if we do it from 1 to 2 to 3 it is anticlockwise so this configuration is this right fourth group is in the vertical line so this should be S.

And this S configuration is at point number 5 so we should name this as 5S so this completes the IUPAC name of this particular compound. Hope this is clear to you so for you I would like to give one problem related to this as a homework. Take this molecule and try to write the IUPAC name of this molecule considering the stereochemistry of the chiral centers right. This also another spiro compound and you have 2 chiral centers here and this point is the axially chiral center.

So you need to identify the chirality's of those 3 different chiral centers. Now I would like to move to the next part of the problems where we will try to identify the number of stereoisomers that are possible for different types of molecules.

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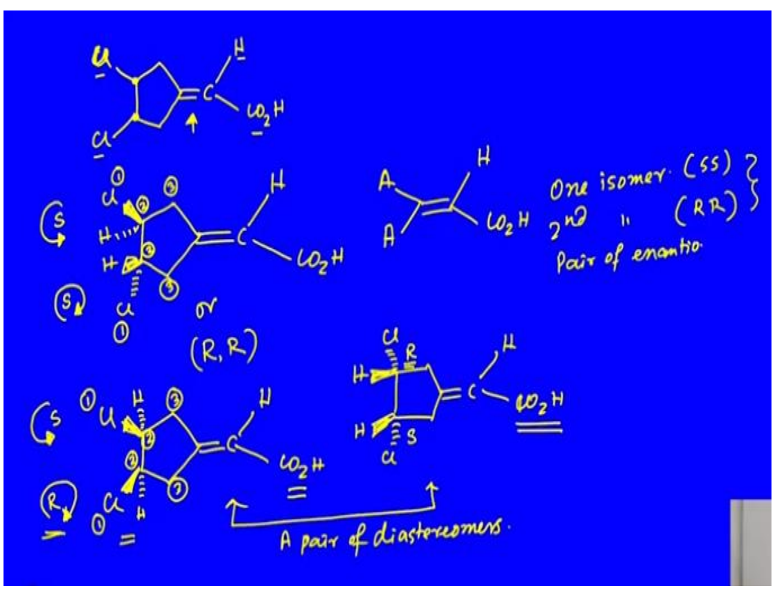

So in this molecule what we see is the C-C double bond and you have 2 different substitutions here. And you have 2 substitutions which are in terms of atoms they are same because they are chlorine. But you see that they may have a different stereochemistry at these 2 points. So let us try to see what are the possible enantiomers of this compound? So this is one of the isomers of this compound where you have hydrogen and CO2H in this direction and you have chlorine up and chlorine down.

So if we see at this molecule this chlorine gets priority 1 this carbon gets priority 2 because this is then connected to chlorine and that carbon gets priority 3 because it gets connected to a second carbon. So here we look at it 1 to 2 to 3 is anticlockwise so it is S and hydrogen is it at the back. In this particular case this is 1 that is 2 and this is 3 so it is 1 to 2 to 3 is clockwise but then we are looking at it from the direction of this so this is S.

So both of them being S this has only one isomer because for this group what we have here is like a double bonded carbon with hydrogen and CO2H and 2 groups are same. So this is only one isomer the only possibility is to have this as SS or RR. So this is the SS form and that is the RR form so you have 1 isomer which is SS the other isomer is RR and there is no geometric isomer possible for this.

But then when we have the opposite one which is like this, both the chlorine atoms are above the plane. So we write the priorities as 1, 2, 3 so 1 to 2 to 3 anticlockwise is S and here it is 1 to 2 to 3 is clockwise so it is R. So now we have one possibility of having both R group which is more prior here and more prior there on the same side. Or we have another possibility of having the molecule like this where these groups are interchanged that is this.

So here it is SR where R and CO2H are on the same side here it is RS where R and CO2H are in the opposite side. So this 2 are a pair of diastereomers and these are 2 different isomers which are RR and SS. So they are pairs of enantiomers.

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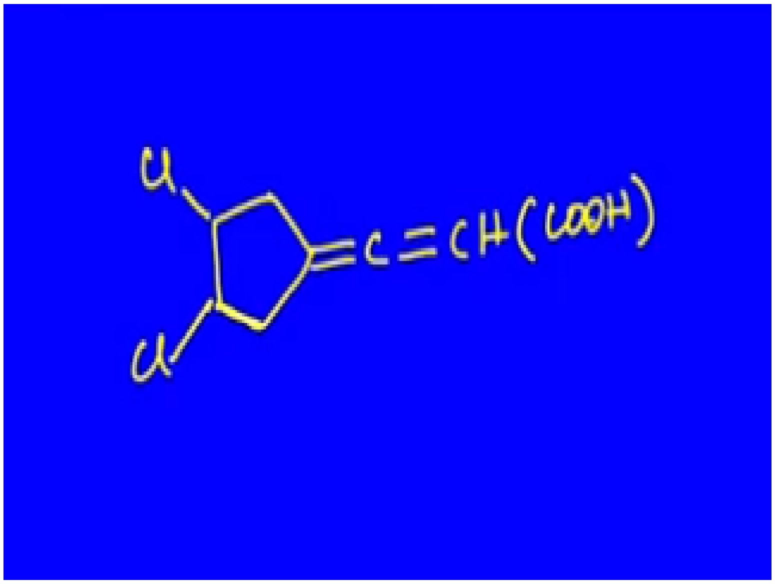

In the same way I would you to draw the possible stereoisomers of this compound. And find out which one of them are enantiomers diastereomers and whether there is any meso compound that is possible in this case. Now we would like to move to the next part which was discussed in the last couple of lectures. The topocity of the different atoms and faces so, I would like you to find out the topocity of the hydrogens that are marked here.

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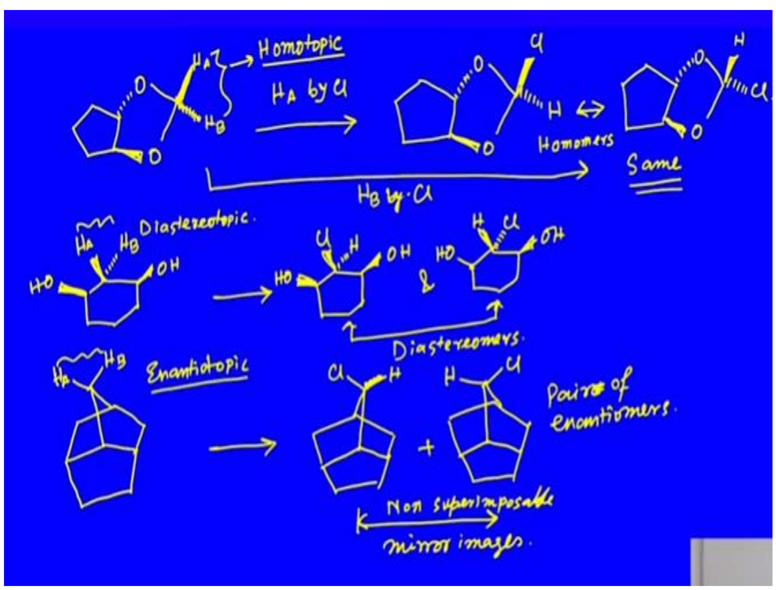

One compound is this one and other compound is this molecule and then third compound that I want you to try to find out the topocity of the hydrogens are is this one. So how do we find it out? We first try to replace one by one replace HA by suppose Cl and we get this molecule. And if we replace HB by Cl we get this molecule. So if you look at these 2 molecules carefully what we see that these 2 compounds are same.

So these compounds are to be called as homomers therefore those 2 hydrogens are to be termed as homotopic. Let us try to see what happens if we replace this HA and HB separately by chlorine. We would get 2 different molecules. So what we see here are these 2 are chiral compounds but they are a pair of diastereomers because they are not related by any mirror image.

So these 2 hydrogens are diastereotopic so now if we try to do the same operation on these 2 hydrogens we replace them one by one by chlorine let us see what happens? These 2 are non-super imposable mirror images therefore these 2 are pair of enantiomers therefore these 2 hydrogens are enantiotopic right. So I would like you to find out the topocity of different hydrogens.

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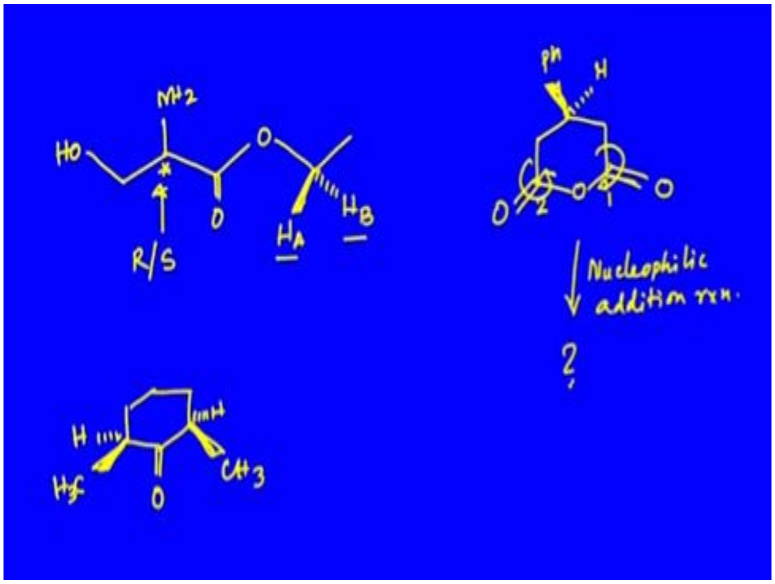

I am giving you 2 examples here for your homework to find out the topocity of those 2 hydrogen atoms considering the chirality of this which is not identified. So it can be both, R or S and then in the next homework you should try to find out the topocity of these faces. As you see here it is a ketone and this ketone as 2 faces one is from the top of this projection and the other one is from the bottom of this projection.

So find out the topocity of these 2 faces. The next example or next homework is this molecule this has 2 C double bond O groups namely 1 and 2. Find out the topocity of those faces here whether they are enantiotopic or diastereotopic. So what is the way to find out? You try to do a nuecleophilic addition reaction as we have discussed in the previous class and try to find out what would be the product. And from that you should be able to identify what are the topocities of those 2 faces. So we will continue from here in the next class thank you.