Structure, Stereochemistry and Reactivity of Organic Compounds and Intermediates: A Problem-Solving Approach

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Lecture 10

Conformational analysis of Perhydrophenanthrene

Hello. Welcome back to this course on Structure, Stereochemistry and Reactivity of Organic Molecules and Intermediates: A Problem-Solving Approach. In the last lecture, we have, we are discussing the conformation analysis of bicyclic cyclohexane systems. We have taken the decalin as our example and we have studied the conformations of trans and cis decalin and then their derivatives as well as their reactivity.

We will come back to these decalin systems later on when we solve the problems after we finish up this topic that is the conformational analysis of bicyclic and tricyclic cyclohexane systems. Today, we will discuss the tricyclic cyclohexane systems.

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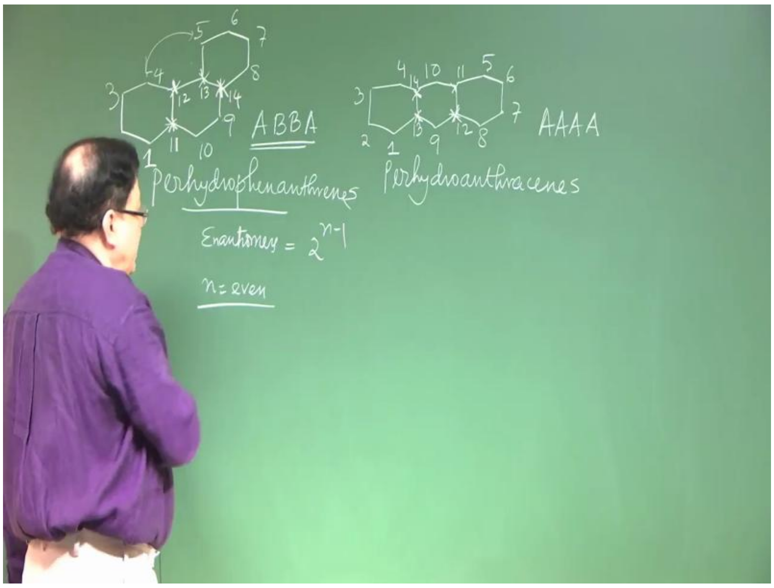

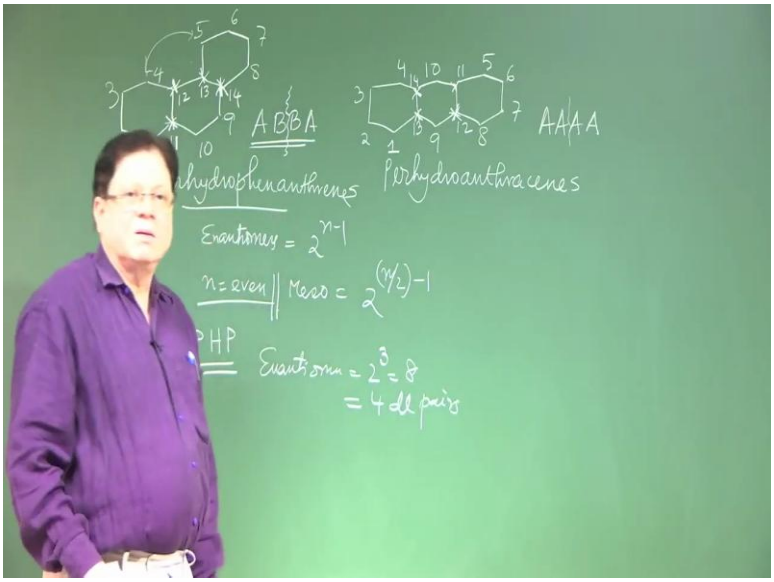

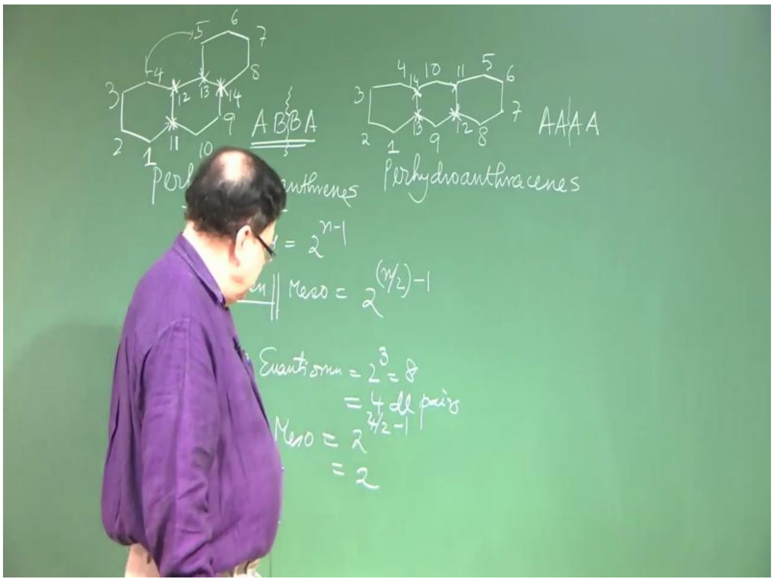

And the molecules that we will choose are one is called Perhydrophenanthrene which is obtained by complete hydrogenation of phenanthrene moiety. And so, this will be called Perhydrophenanthrene. And we will also discuss the other system which is derived from anthracene moiety, hydrogenation of anthracene, complete hydrogenation of anthracene. So, that will be called perhydroanthracene.

Now, actually perhydroanthracene can exist in several diastereomeric forms, so also the Perhydrophenanthrene. So basically, we are discussing the perhydroanthracene and the perhydrophenanthrene. Now let us try to figure out that what will be the number of diastereomeric forms that each molecule can have.

Now, we for that we have to identify how many stereogenic centers are present in this system. So, let us take perhydrophenanthrene. So, you have one center here; another center there; a third one here and the fourth one there. So, these are the four. And we know that if there are 4 stereogenic centers like the stereogenic center that we are talking about is the sp3 stereogenic centre that means the erstwhile chiral center. So, that generally give rise to 2 to the power n stereo isomers.

However, since some of these stereogenic centers are similar so their number of stereoisomers will be less than when they stereogenic centers are all different. This is basically where are these similarities? Like this center is similar to that center. And this center I am pointing out and this center, they are also similar. Rather than saying this and that let us try to number it.

The numbering system that is followed IUPAC numbering system and that is based on the perhydrophenanthrene. When we number perhydrophenanthrene, we know that these centers are actually 9, 10 positions. And these centers which are called the bay these two, they should be 4 and 5. So, you have to number it in such a way that the bay region get 4, 5 numbering.

So, that means you have to start from here 1, 2, 3, 4, 5, 6, 7, 8, 9, 10. So up to that point is fine, 9, 10. And then you continue this. So, this is 11; that is 12; that is 13 and this is 14. So, the stereogenic centers are the C-11, C-12, C-13 and C-14. C-12 is essentially similar to C-13 position the C-3, carbon 13 position. And the C-11 carbon is also same as similar to C-14 carbon. So, that is called ABBA type system.

And if you do the same thing here; in anthracene the numbering can start from anywhere. So, you can call it 1, 2, 3, 4 then 5, 6, 7, 8. You know that anthracene these two positions the middle ring positions are 9, 10. So, you have to satisfy that- 9 and this is 10. Then this is 11, 12, 13, 14.

So, but this will be called AAAA type because all the stereogenic centers; here also this C 11, 12, 13, 14 are the stereogenic centers- the sp3 stereogenic centers and but here all the four are having same type of similar type of atoms connected to them. So, that is called AAAA type and this will be ABBA.

Now, when you have the more similarity you have the number of isomers will be less. The more similarity you have that lowers the number of stereoisomers. Now, there is some formula which is existing for this type of system ABBA and that says that enantiomers, the number of enantiomers for ABBA system equals 2 to power n minus 1.

2 to the power n minus 1 provided n is even. This is for n is even. Here n is even because the number of stereogenic centers are 4. So, this is the number of enantiomers. 2 to the power n minus 1.

And number of meso compounds because there will be now chances of meso because you will have the presence of plane of symmetry. Here also presence of plane of symmetry is possible. So that will reduce the number of stereoisomers in the active form and some of them will become meso as a result.

So, the number of meso is basically 2 to the power n by 2 minus 1 so when n is even. So, we are dealing with here n is 4. So, we can say the number of enantiomers here will be for perhydrophenanthrene if I write it perhydrophenanthrene PHP. So, enantiomers is equal to 2 to the power 4 minus 1. So, 2 to the power 3. That is equal to 8. So, that says that there are four dl-pairs. 4 dl-pairs, correct?

And the number of meso will be 2 to the power n by 2. That means 4 by 2 minus 1. So, that makes it 2. So, number of meso is 2 and the number of enantiomers is 8 and that will exist as 4 dl-pairs. So that is the; so, we have to identify what are those? We will come back to the perhydro; perhydroanthracene.

Obviously, we have less than here the number of, total number of isomers will be 8 plus 2, that means 10. And in perhydroanthracene that will be less because it is AAAA type. We will come back to that problem once we go through phenanthrene, perhydrophenanthrene system.

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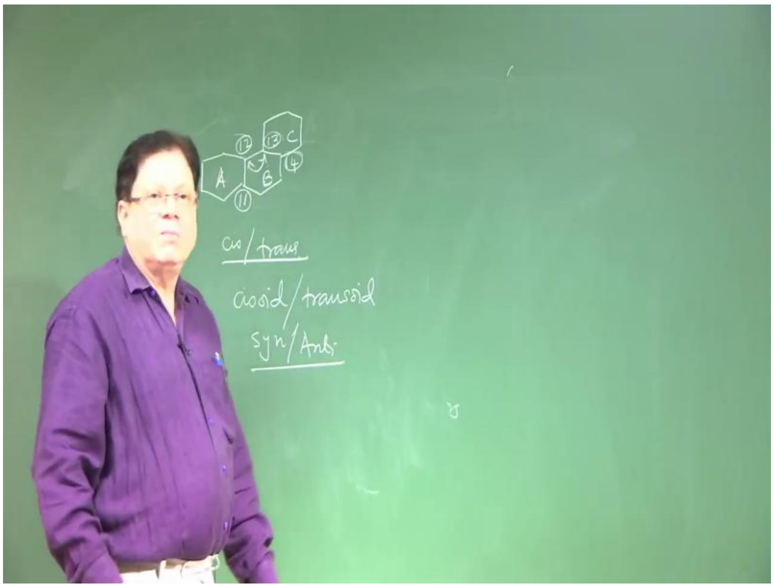

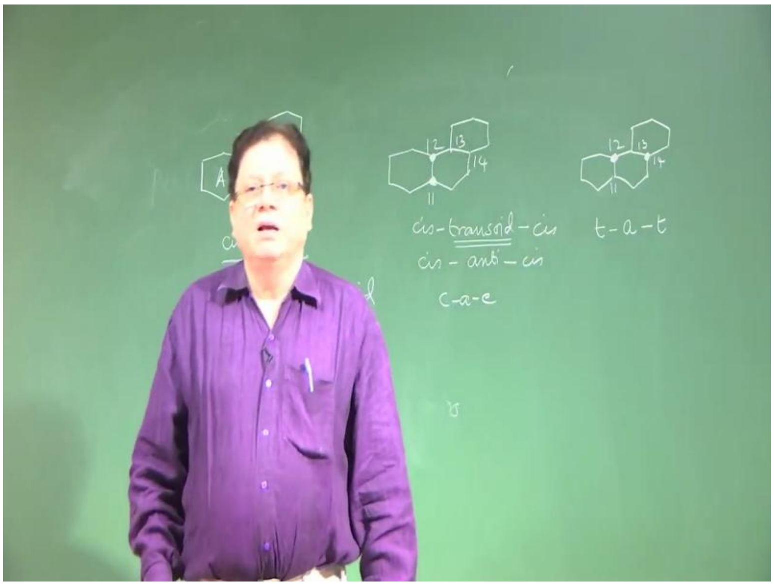

So, we will start with the perhydrophenanthrene. Try to draw the various conformations based on the ring junction stereochemistry as well as; see there are basically two types of relative stereochemistry involved here. Again, I write. This is 11. This is 12. This is 13 and this is 14. And there are the relationship, steric relationships exists between C-11 and C-12. So that could be that means the ring fusion, the ring junction basically or the two rings where they are fused, that is 11, 12 position and that is also 13 and 14.

So, one so, these 11, 12 the possibility are basically cis or trans. So, that is one type of stereochemistry, relative stereochemistry involved at the ring junction. And the other relative stereochemistry that is existing between 12 and 13.

Remember 13 is basically present if I call it A ring; this is B ring and this is C ring. 13 is present in the C ring and B ring. It is common to B and C whereas 12 is common to A and B. So, 12 and 13 are basically, they do not belong to a particular ring. They belong to different rings.

And so, their relationship is denoted by cisoid or transoid or in our earlier nomenclature system, they can be called as syn and anti. Syn or anti. I will give you some example. That will make it clear. Like suppose I have on this ring junction I make it say cis.

And remember, I think I have already mentioned that when I put a because the hydrogens are not shown in the structure. That is number one. Number two is that these hydrogens did not be shown and there is no stereochemistry involved here. There is no stereogenic center here.

But these centers are stereogenic center. So, there is a question whether the hydrogens are up or down. If it is down you do not have to do anything. So, if nothing is mentioned that means the hydrogen is down. If the hydrogen is up then you have to make it a dark circle. That means the hydrogen is up at that position.

So, if I have this type of molecule, I have the hydrogens up here. And obviously nothing is mentioned here. That means the hydrogens are down there. So, this will be called a cis then. So, 11, 12 is cis. Then 12, 13 is transoid. So, that can be so, that is basically transoid. That is the correct present-day nomenclature. And then 13 and 14 is again cis. So, this will be called cis-transoid-cis. So right now, for simplicity, we call it as suppose anti. And so, that will be cis-anti-cis. And that can be abbreviated as c-a-c, cis-anti-cis.

So, similarly, we can have; suppose I draw these. Only these two are darkened. So, this is 11; this is 12; this is 13 and this is 14. So, how do you describe this molecule? This is basically 11, 12 is trans. So, that is t. And then 12 and 13 is also trans. So, because it is beta and the 13 hydrogen is alpha. So, anti, t-a. And then, 13 and 14 is also trans. So, this is a t-a-t molecule. So, let us try to find out how many are possible.

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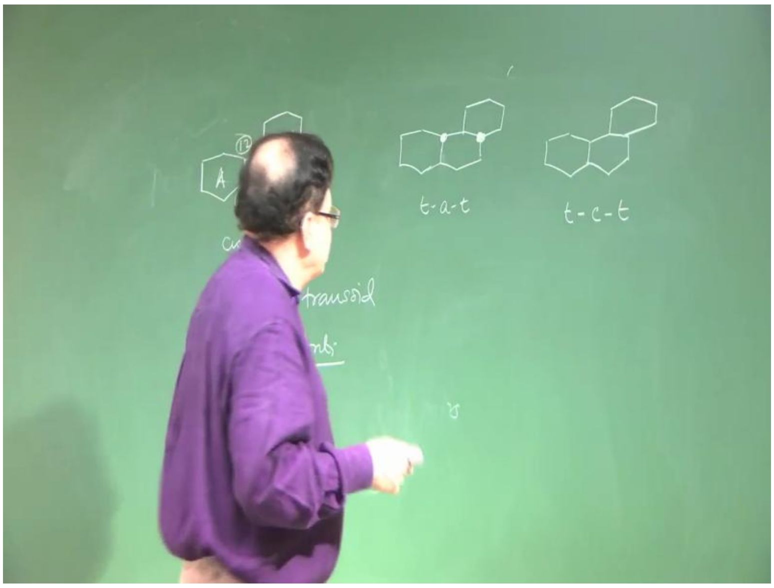

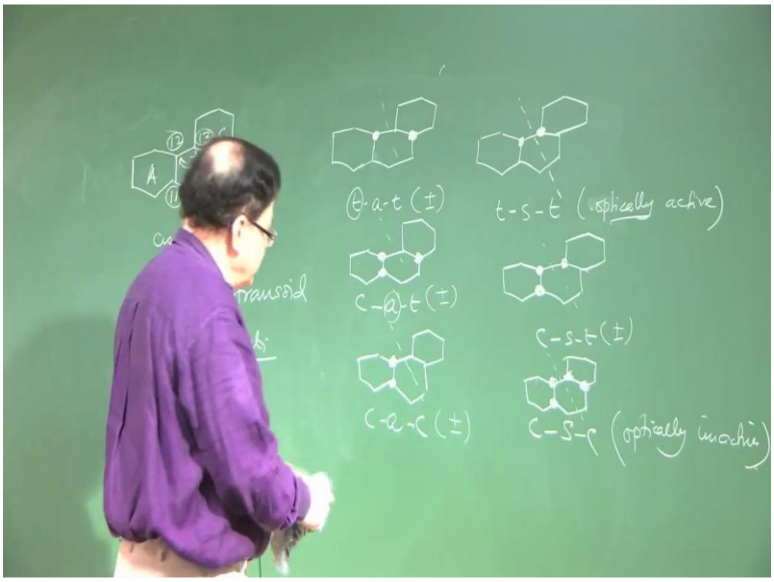

So, maybe start from the very beginning. So, first let us draw; let us assume that we will have all trans system that I have already just drawn a few seconds back. So, this will be t-a-t. This will be t-a-t. And then you have if you go systematically then that will be better. Do not do it in a haphazard way, in a random way.

So, if it is first is t-a-t means you are actually having an all trans type system. So, the other, the next one that should come in your mind is t-c-t. That means trans, and then cisoid and then trans. But here because we are using the syn-anti nomenclature so we can say that this is t-s-t. Correct nomenclature is trans, then cisoid and then trans. t-s-t: trans-syn-trans.

If I have to do that, so this is this make it 11-12 trans. And then I have to make a syn orientation that means cisoid orientation. So, I have to make it bold. And then a trans. So, this is the molecule- t-s-t. So, what will be the next one that we should think of is we make one as cis.

So, c-a-t. If I have c-a-t, then let us draw that. See we are drawing the planar formula and/or the planar structure which is obviously not the conformation of the molecule. We will convert this into the conformation once we are through with the number of isomers or depict the number of isomers in the planar structure.

So, the next is c-a-t. That means, cis-anti-and trans. So, correct name is cis-transoid-trans. So, this is cis that means we make it both bold. So, that makes it cis. Then, anti. So, I have to have it have it alpha hydrogen and then trans that means it should be bold. So, that will be c-a-t.

Then what will be the next one? The next one is that you convert, you make it syn here. That means cisoid. So, that will be that will be c-s-t. So, c-s-t. So, we have to make it cis; that means both bold.

Then you have to make it syn; that means again these two should be bold. And, then trans. So, this is the planar structure of the c-s-t isomer. So, 4 are gone. So, what will be the our next one?

So, see here we have both trans system. Here we have one cis, one trans. So, one type of relative stereochemistry still there and that is cis and then also that the other one is also cis. And in the middle, you have either anti. So, c-a-c.

So, that will be in the planar structure that will become cis. So, that will be both bold. Then anti and then cis. So, this is the one. c-s-c. And then you can tell what is left? That is c-s-c. c-s-c means this is bold; that is bold. Sorry, let us complete this. This is bold and that is bold.

So, these are the 4 diastereomers we can say; 4 diastereomers. And there is a possibility that that they can exist as dl-pairs or there is a possibility that they can be a meso. So, then it will be only a single diastereomer. So, we have to find out that.

Now, there is a you can arrive at the conclusion by looking at that this planar representations by finding out whether they have any plane of symmetry or not in the plane structure. That is planar structure.

However, with a word of caution that sometimes you can see an apparent plane of symmetry here but which may not be there in the actual molecule. We will, we have seen this type of thing in cis-1, 2-dimethylcyclohexane.

If you consider it as a planar structure, then you will have a plane of symmetry. And that gives; that tells you that cis-1, 2-dimethylcyclohexane exists as meso. However, in the actual scenario what happens? Because these two methyls are actually one axial one equatorial, so there cannot be any plane of symmetry. And then molecule never adopts the planar configuration.

So, what happens here? That flipping develops the mirror image. So, it exists as a non-resolvable dl-pair. However, the optical inactivity because non-resolvable dl-pair or meso, both will show 0 optical rotation. So, your conclusion that they will be optically inactive that will remain the same.

So, with a word of caution, first you make it whether they are optically active or they can be optically inactive by looking at the plane of symmetry. This does not have any plane of symmetry. So, that should exist as a dp-pair. The plane of symmetry we are talking about is basically that has to go through this.

And this has a plane of symmetry. So, that should exist as a optically inactive. We will find out whether it is a real meso or it is a non-resolvable dl-pair. Because both will not show any optical rotation.

This one is c-a-t. There is no plane of symmetry. So, that should exist as plus-minus. Then this is c-s-t. That is also devoid of any plane of symmetry, so that is plus-minus that means dl-pair. So, then c-a-c that is also should exist as a plus-minus mixture and c-s-c obviously that will have an apparent plane of symmetry.

I use this word apparent because here you never know what are the orientations of these hydrogens. Because if one is equatorial and other is axial, then you will not have any plane of symmetry. However, in the planar structure it is showing a plane of symmetry. So, the better word is an apparent plane of symmetry. So, that will be optically inactive.

So, we will not go through all. We will not go through the conformational analysis of all. What we will do? We will take some of these. We will discuss some of these molecules and discuss their conformational analysis and their number of gauche-butane interaction. So, what will be the overall excess energy over the cyclohexane system. Cyclohexane chair form.

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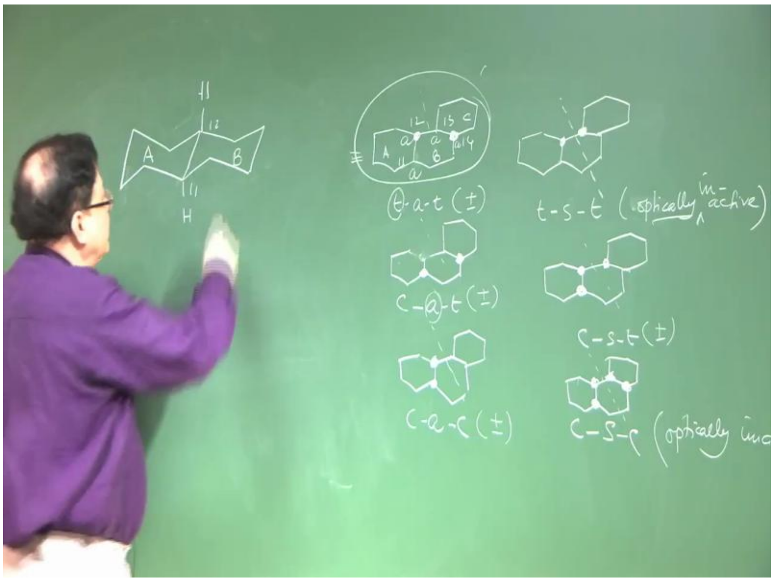

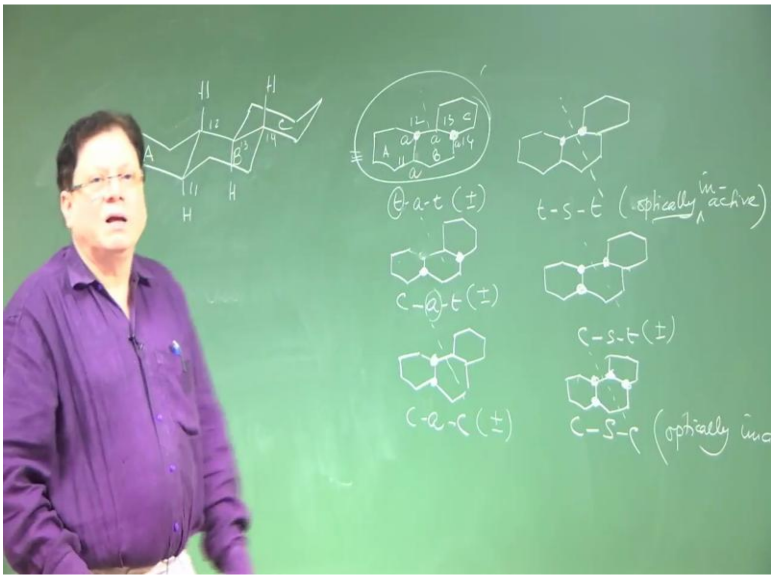

So, let us talk about; let us take any one of these. Say, t-a-t. Let us talk about this molecule. First of all, we have the formula. Adopting the formula for n equals to even for ABBA system, we have seen that it should exist as 4 dl-pairs and 2 meso according to that formula.

Here meso means I am saying that they are basically at this stage we should write optically optical inactive. Sorry. This is optically-inactive; optically inactive. So, optically inactive. So, there should be 2 optically inactive forms. Yes, that is correct. That was according to that formula and then there will be four dl-pair. Yes, there are 4 dl-pairs. So, I think we are not missing any of the isomers that is for sure.

Now, let us try to draw the conformation of this molecule this t-a-t. Now, how to proceed by drawing to draw these molecules? Better you know the hydrogens reside at 11, 12, 13 and 14 positions. Try to assign the axial-equatorial orientation of these hydrogens.

Now, 11-12 has a trans ring junction. If for a trans ring junction you know the hydrogens have to be di-axial. So, hydrogen has to be di-axial. So, this hydrogen whatever is here at the alpha so that will be axial. So, this hydrogen will also be axial. And then 12 and 13, they are actually 12 and 13 are belonging to the B ring. But they are not common to A or C.

Like the relative orientation I talked about that they are not actually representing any ring junction. So, 12 and 13 belonging to the B ring and we know that basically they are having a 1-2 relationship, if we look at only at the B ring. This is the A ring. This is the B and this is the C.

So, B ring: this is 1-2 relationship, 1-2-trans. That means 1-2-trans means either both are axial or both are equatorial. So, if this is axial, then this hydrogen should also be axial. And if this hydrogen is axial, this is now, this is the beta hydrogen. So, that will be because this is now trans: 13 and 14. So, that will be also axial. So, it is all axial; hydrogens are all axial.

Again, I repeat. This is trans. So, both hydrogens have to be axial. 12 and 13 are trans. So, again because this is axial so that will be axial. Now, this is with relation to the B ring. Now, when we are talking about this axial here that is in the B ring. And then this is 13 and 14. So, that is also a trans ring junction. So, both hydrogens have to be axial.

So, let us draw the structure. First draw the A ring. Now, first draw the B ring. The best way is to draw the B ring. So, this is your ring B. Now, the axial hydrogen is at the 11 position. So better make this as 11. Do not make this as 11 because the hydrogen becomes beta. You are starting with a alpha axial hydrogen. So, that means this hydrogen is here. So, that is 11 and this is 12. So, this hydrogen is axial. So, complete the ring, the A ring. So, this is your a ring. And then complete the C ring.

The C ring is again this is your 13. This is your 14. Do not be in a hurry. This has to be done in a very systematic manner. So, 12 we have done. Now, 13 the hydrogen is axial, alpha-axial. So, find out those hydrogens. 14 hydrogen is beta axial. Now complete the C ring. So, the C ring is basically this; ABC.

Now, one point to remember is that this is a tricyclic system. If you have any trans ring junction; any at least one trans ring junction in this tricyclic system then the whole molecule becomes rigid. You cannot flip it.

So, what I am saying that if A and B having a relationship of trans or A-B and B-C are having trans relationship, so either both having trans relationship or at least one trans relationship exists, then the system becomes rigid. So, this is a rigid system. You cannot flip this. So, if you cannot flip this then it is a rigid molecule and there is no question of flipping gives mirror image. That is not possible here. Flipping is prohibited here.

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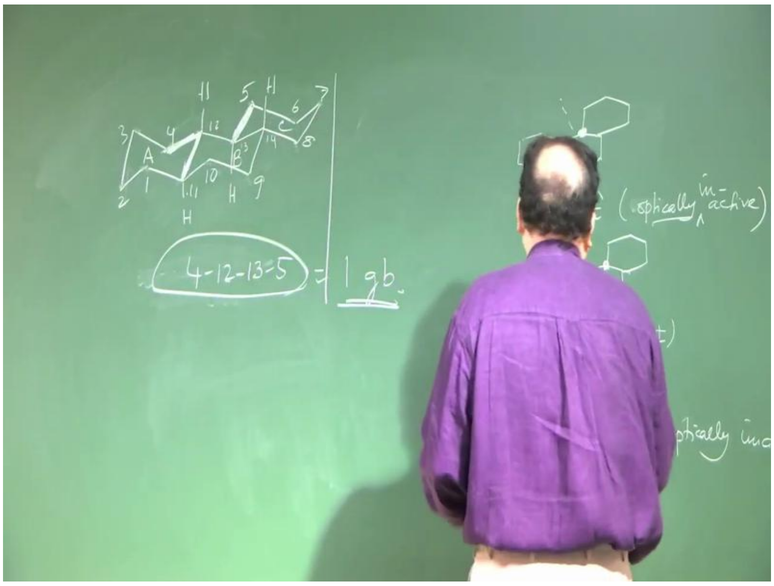

Now, there are two things that remain that how many extra gauche-butane interactions that you are incorporating into this system. You know that in trans-decalin system, you are not incorporating any extra gauche-butane in the trans system. Because all the; these carbon-carbon bonds are basically in the transoid form.

So, you are not all means, you are just not considering a bare cyclohexane chair. You are not considering that that when the cyclohexanes are fused together then whether you are incorporating any extra. Remember extra over the already present in a cyclohexane chair.

So, if in trans-decalin we know that we are not incorporating any extra. So, here these two are A-B is trans. So, you are not incorporating any extra. B and C are also trans. So, you are not incorporating any extra butane units. However, there is one situation you have to be so, ring fusion does not give any because both are trans.

However, there is one extra butane unit that comes because of this disposition of these A and C rings. The disposition of A and C rings are such that this bond and this bond, they form a butane unit which is not incorporated in a trans-decalin; which is not due to a trans-decalin system. So, that is beyond the trans-decalin system.

Actually, beyond the decalin system. This is present in all the perhydrophenanthrenes. This will be present in all perhydrophenanthrenes irrespective of whether this is chair or in the boat, whatever. Irrespective of that this unit is always present.

However, see our numbering system has 1, 2, 3, 4, 5, 6, 7, 8, 9, 10. No. Actually, this is 1; 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12. 1; just a second. Let us try to number it. So, if this is 1, 2, 3, 4 then 5, 6, 7, 8, 9, 10 and this is 11, 12, 13, 14. This is clear. So, the butane unit that we are talking about is C4, C12. Do not write the carbon; 4, 12, 13, and 5.

So, this you have to be careful. Even if they are in trans ring junction, you have to be careful whether this is causing, these butane unit is present in gauche form or not. And these are certainly they are forming a gauche butane unit. There are many ways to look at this. One way is that the anti to this carbon-carbon bond is this ring-junction bond.

So, you know that there is only one anti bond that can be present, okay, for a 1-2, system. So, this has to be in gauche. And it looks that they are not anti to each other. So, that is the gauche-butane unit. So, one extra gauche-butane interactions is present in this system. So, that is important.

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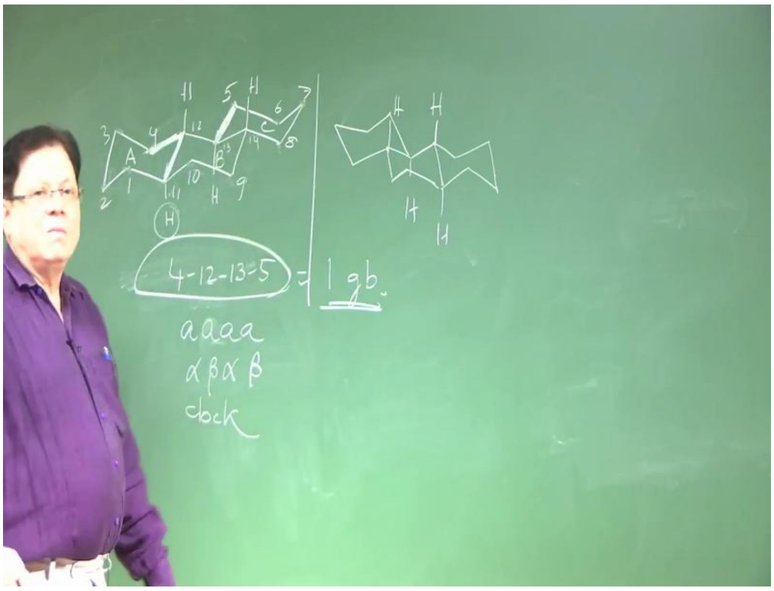

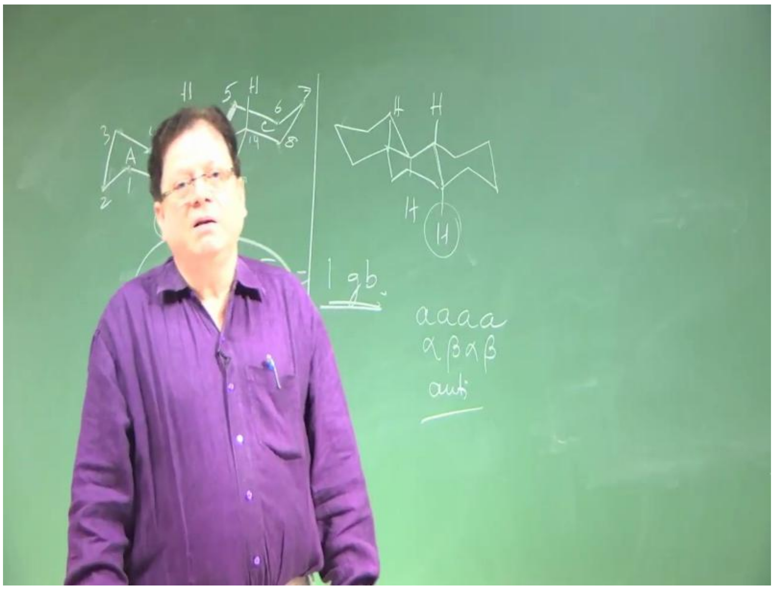

Let us quickly do another one. Suppose the t-s-t, the t-s-t. Okay, we have not yet figured out whether it is optically active or not. In order to do that what you have to do? You have to draw the mirror image of this. So, that is this one. And then let us complete this and then this is the mirror image of this form. And put the hydrogens now. Hydrogen here; hydrogen there; hydrogen here; hydrogen there.

Now, how to compare these two systems? You know my lecture in stereochemistry topic, this stereochemistry subject. That NPTEL stereochemistry lecture series, we have given a mnemonic device to compare the chair forms of cyclohexanes. Irrespective of whether it is a mono cyclic or bicyclic or tricyclic. We are going to adopt this mnemonic.

What you do? You first figure out that I pick out these hydrogens, the ring junction hydrogens say this one 11, 12, 13, 14. And then try to look at their equatorial-axial nature as well as try to look at their alpha-beta nature. And then try to find out that if I go from one end to the other end by the shortest route, then I am what is the direction of my movement. So, these three.

The first one for this is that you have to check the axial-equatorial nature of this. So, here if you go from C11, then C12. So, this hydrogen is axial then hydrogen is again axial, axial, axial. So, all are axial, axial, axial, axial.

Now, if you start from this C11 and going to C14, then the alpha-beta nature runs like this. That this is alpha; then this is beta; then this is alpha; and then this is beta. And the direction is clockwise. And if you do the same thing here. First you have to fix the axial but here all 4 are axial so you can start from any end: axial, axial, axial, axial.

And to maintain parity here alpha, beta, alpha, beta; you are seeing that I should start from here and then go in this direction. So, if I do that then this is alpha, beta, alpha, beta and the direction is now anti-clockwise. The direction is anti-clockwise. And if that be the case then what happens? That one is different, then they are mirror images of each other. Non-superimposable mirror images of each other. That means they are non-superimposable. So, that makes it optically active.

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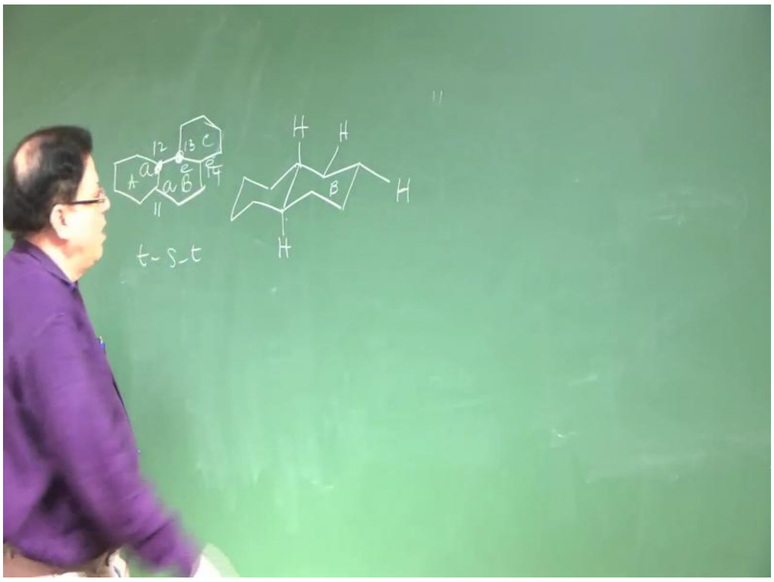

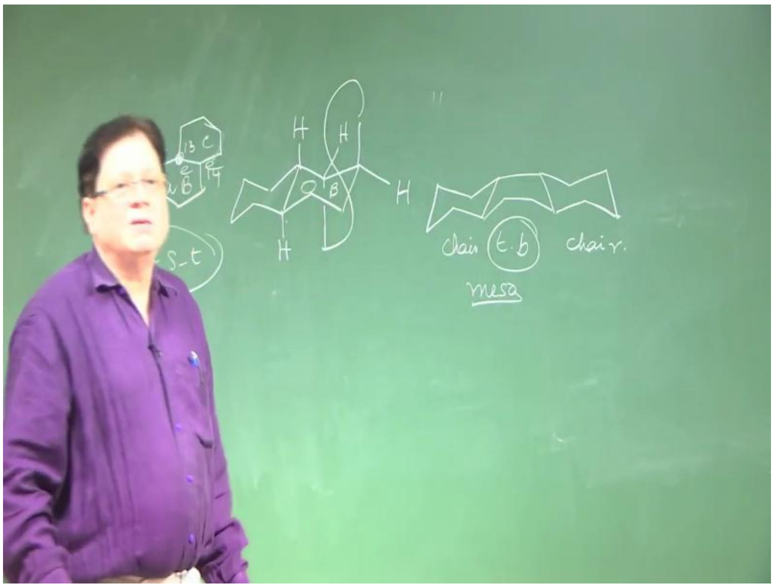

Then, let us quickly do another one: t-s-t. What is t-s-t? Sorry. T-s-t that means, you have this and then this; t-s-t. So, this is t-s-t. Trans and then cisoid and then trans. So, this is my 11. This is 12. This is 13. And this is 14. So, again first assign the alpha-beta; this axial-equatorial nature depending on the ring junction's stereochemistry.

So, because it is trans, so this is axial and this is axial. Both are axial. Then this is 1, 2-cis relationship. So, that should be equatorial. And then the hydrogen, in order to make it a trans ring junction should be equatorial. Now, that puts us into a problem. What is the problem?

The problem is not between this A and B ring. The problem is basically how to draw the B and C ring with the hydrogens in the di-equatorial form because we know that trans ring junction exists only when for a trans ring junction, the hydrogens at the ring junction should be di-axial. They cannot be di-equatorial. Why?

Because then you cannot connect; you cannot complete that if the hydrogen occupies di-equatorial relationship, then the di-axial relationship should be occupied by the ring bonds. And then you cannot connect the ring bonds because one is going up another is going down. And if there is no possibility of connecting these two ends by only 2 carbons that were remaining at that time.

So, basically now you see that this there is a problem. You cannot draw this molecule in perfectly chair form. All 3 cannot be in the chair form. And if you try to draw that; let us see. If you try to draw that; see I said that this should be your B ring. If you put the B ring in the chair form. And then this is your A ring.

So, hydrogen 11; this is hydrogen 12, beta. And then your 13 hydrogen is equatorial. So, this will be here and this is the equatorial that will be there. And now you have to complete the ring from these two which is not possible. This is not possible. The ring cannot be completed.

So, what happens? This actually adopts the ring B adopts a boat conform skew, a twist boat conformation here. And then you can draw the other rings in the chair form. So, this is the conformation of the of this t-s-t molecule. The middle one is in the twist boat. So, that is twist boat. And this is your, this is chair and that is the chair form. So, this is something a little bit different.

And this is; because it is a trans ring junction. So, I said that if one trans ring junction present then you cannot flip this molecule. So, flipping is not possible. However, if you draw the mirror image you will see that they are superimposing on one another. They are same basically. So, that is a meso compound: t-s-t.

And the energy is basically here the energy will be the energy that is present in a twist boat conformation. Maybe there is time for one more. Let us do that. We will take the another one which is c-c-c. I think that it will be interesting.

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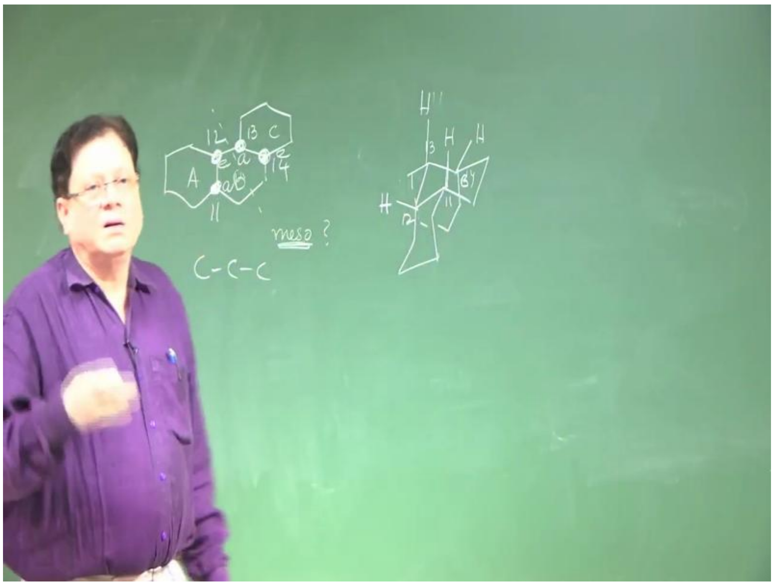

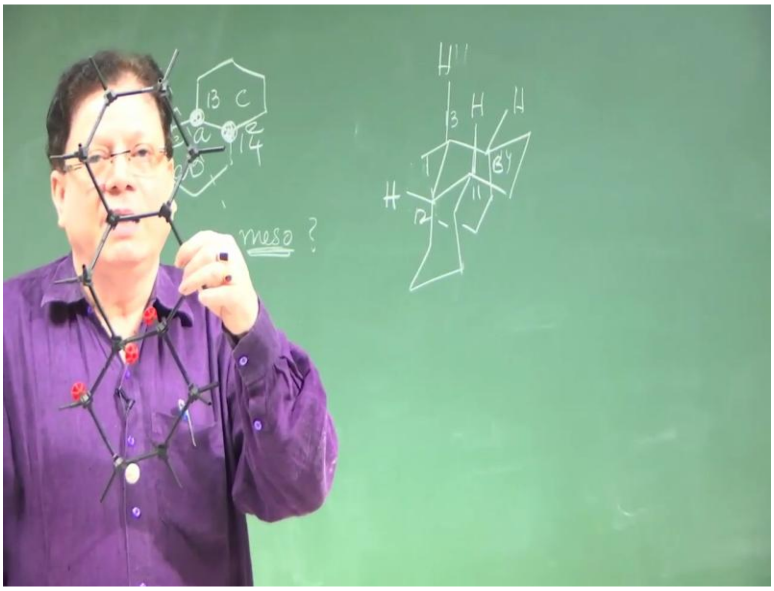

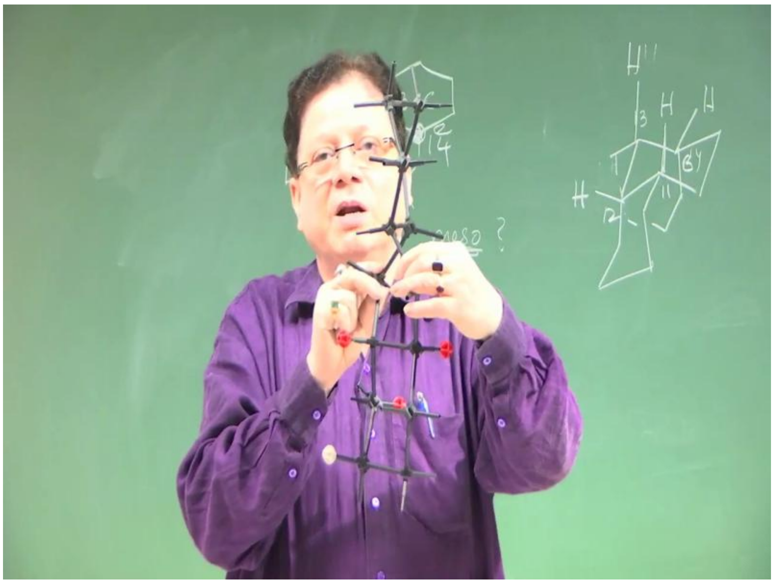

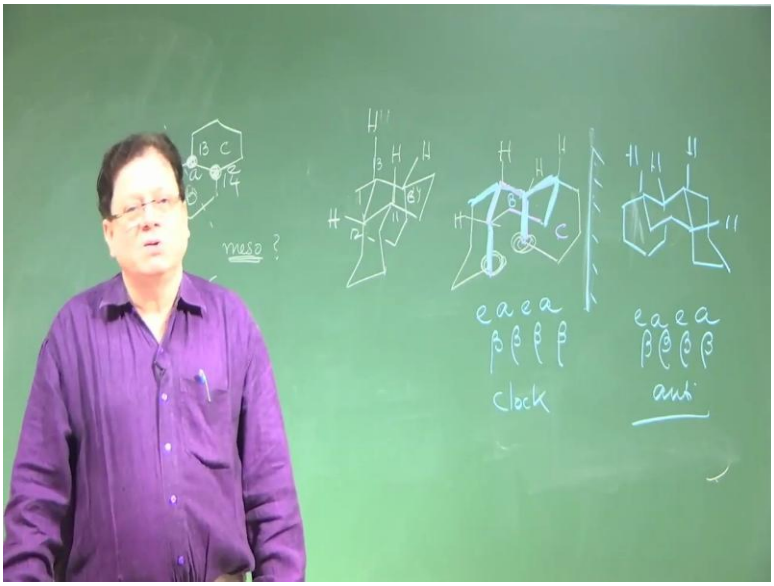

So, c-c-c. That means this is cis, this is syn and this is cis. So, 11, 12, 13, 14. Now, let us try to draw the confirmation ABBA. The planar confirmation predicts that it should be exist as a meso. So, now the question is whether it will be a real meso or a non-resolvable dl-pair.

So, let us try to find out. Again, I say that first you try to assign the axial-equatorial orientation. So, this is a cis ring junction. So, you have the option here. Now, you can start with; this is axial. This hydrogen is equatorial because this is 1, 2 relationship. Then this is 1, 2 relationship. So, that will be axial and that will be equatorial. So, here it will be axial-equatorial, axial-equatorial or the vice versa, equatorial-axial, equatorial-axial.

So, let us draw the B ring first. So, this is your B ring. The C11 we have assigned an axial orientation and is beta. So, better put the 11 carbon, the 11 position at this; assign 11 number to this carbon. So, the hydrogen becomes beta-axial so that it matches with this. And now you complete the ring.

This is cis ring junction. So, 11, 12 and then you have 13 and 14. 13 and 14. So, 13 hydrogen is beta-axial. So, 13 hydrogen is here and the 14 hydrogen is beta-equatorial. So, that will be in this direction. So, now the other ring unfortunately false is behind this and you cannot show it as a, you cannot show it in the chair form because it is actually facing; you are facing this ring like this.

And the projection of this ring, the ring which is shown here will be like a plain hexagon. And that is what is. But that does not mean that it is not existing in a chair form. Because if it is viewed in this direction, you see that this is actually existing in the chair form.

Sometimes what happens? Because of the orientation, it looks like that it a six membered ring. It is a plain hexagon. But actually, this is present in a chair form. You can this is a little bit clumsy. You can make it little bit better by having by making this 11 as equatorial. If you start from here equatorial-axial, equatorial-axial then you could have started in this fashion.

See, this is the 11, equatorial-axial. And then equatorial-axial. So, the next ring at least they are not overlapping on each other. Their projection is not overlapping. So, at least this is better; this is a better representation of that.

Now, how many extra gauche butane units it may have? You can quickly because there is a cis-decalin system. There are 2 cis-decalin systems present. So, that gives you 6, that gives you 3; each cis-decalin gives you 3. So, 3, 3, 6. That will be there. However, the other way to look at this system is that there is this 2 CH2’s which are having a 1, 3 which are in a 1, 3 di-axial relationship.

So, the energy calculation will be based on that either you calculate the interaction energy between these di-axial CH2’s; di-axial methylenes. So, that takes care of this backbone. That takes care of this backbone. Let me try to find out another chalk. Yes. So, that takes care of these backbones.

Now, apart from that, so, either you calculate the interaction energy of these two methylenes, then you do not have to calculate that 6 gauche butane units. If you take that into account then after this you have 2 more and these 2 are basically involving that are present involving other bonds.

Like this is axial. This is the one which we are talking about. Let us see. This bond and this bond belong to the C ring and this appears to be axial to the B ring. So, there is 1 extra here. And there is one more. So, this is the extra additional one. And there is one more additional one and that is; again.

Let me again quickly repeat this. What I am saying that first of all you can look into this system as there are 2 separate cis-decalin systems. So, that gives you 6. Each decalin system gives you 3 additional gauche butanes. So, 6 that comes here. Or you can look at the methylene-methylene interactions. That takes care of this backbone.

Then only if you exclude this backbone, then what is basically remaining is the other one, involving other bonds like this and this one which is not involving that backbone. So, that methylene-methylene interaction plus 2 gauche butane interactions. That gives you, you can calculate that, you can look at the books. That is not the problem. I think that will be; in kilojoules that will be 22 here and then about 7. That is in terms of kilojoules. So, that makes it about 29 kilojoule per mole that this molecule will have the extra energy.

Now, what about the optical activity? Here it says meso. But if you flip it or if you take the mirror image of this. Let us take the mirror image of this. So, this is the B ring. Then, where is you A ring? This is you A ring. And where is your C ring? The C ring will be here. So, put the hydrogens here.

Okay now, very quick we will go through that mnemonic device, apply that mnemonic device that this is suppose we go from here to there to there to there. So, that will be equatorial, then axial, then remember all these relationship with respect to the B ring. Equatorial, axial and then equatorial and axial. And this is; sorry. We complete this. And then beta, beta, and then beta and then beta and then the relationship is, the direction is clockwise.

And if you do the same thing here, equatorial, axial, and then equatorial, axial. Remember this is not; yes, I drawn the mirror image, very sorry. Equatorial, axial, equatorial, axial. Then, beta, beta, beta, beta. But the direction is anti. So, they are non-superimposable mirror image. So, they should be, it should exist as optically, it should show optical activity.

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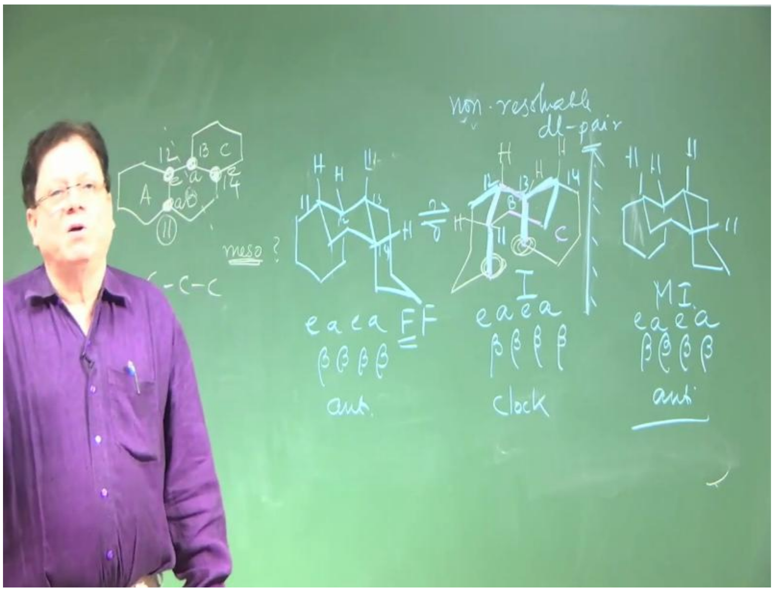

However, the problem is that if you flip this molecule. Let us flip this molecule. Then it will look like this. This is flipping. Remember sign of flipping is this. So, we are now flipping this molecule. The ring B should be like this. And then where are these positions?

So, A will now look like this. This is the A ring. It will look like this. And sorry, not this one. Better number it because that will make it more clean; no chance of mistake. So, 11, 12, 13, 14. So, where is 11? 11 is here because you are taking it up. And then where is 12? 12 is here. Then this is 13 and this is 14.

So, 11-12; so that means this is your ring. Unfortunately, it gives in a, you are looking at a projection which looks like a (cyclo) hexagon. And then 13 and 14. So, where is 13? 13 is here. So, hydrogen, 13 hydrogen was earlier equatorial. Now, it has become axial. This was axial. Now, it has become equatorial. So, this will look like that one. So, this is the situation.

Now, if you adopt the mnemonic again. Then what will happen? You stick to that equatorial, axial, equatorial, axial, equatorial, axial, equatorial, axial. And then your all are beta and then the direction is anti. So, this is your original one. This is your flipped form, flip. And this is your mirror image.

So, what happens? The flipped form becomes (flipped form), FF becomes equal to MI. That means flipped formed becomes equal to mirror image. So, that means that exists as a non-resolvable dl-pair.

So, just to again the conclusion is that in perhydrophenanthrenes there are 2 kinds of stereochemistry that are present. One is at the ring fusion atoms. That is either A-B or B-C which can be either cis or trans. And then there is one more relationship that you have to look into is the relationship at the between the ring junction between the ring junction of A and B that means the 12 carbon and the 13 carbon. 13 carbon is the ring junction of B and C.

So, you have to see the, because they are very close by. So, you have to look at their relationship because there is some IUPAC rule that when you have these tricyclic systems which atoms you should take to denote the relative stereochemistry of the non-fused rings. Here non-fused rings mean A and C.

So, either they are directly connected, the atoms that you are taking or they are connected to the minimum numbers of atoms. Here they are directly connected so that is another question of relative stereochemistry. So, that give rise to the possibilities that you have cis-syn-cis, trans-syn-trans so all sort of possibilities and that we have discussed.

But we have only discussed the conformational analysis of 2 namely we have talked about the t-a-t and then we talked about c-c-c. I think we also talked about the t-s-t. These 3 we have covered. One we have seen that the middle ring B had to be in the twist boat conformational in order to accommodate the ring junction stereochemistry. Thank you very much.