Symmetry, Stereochemistry and Applications
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Module No # 03
Lecture No # 12
Conformational Analysis – Part II

Welcome back to the course entitled symmetry stereochemistry and applications.

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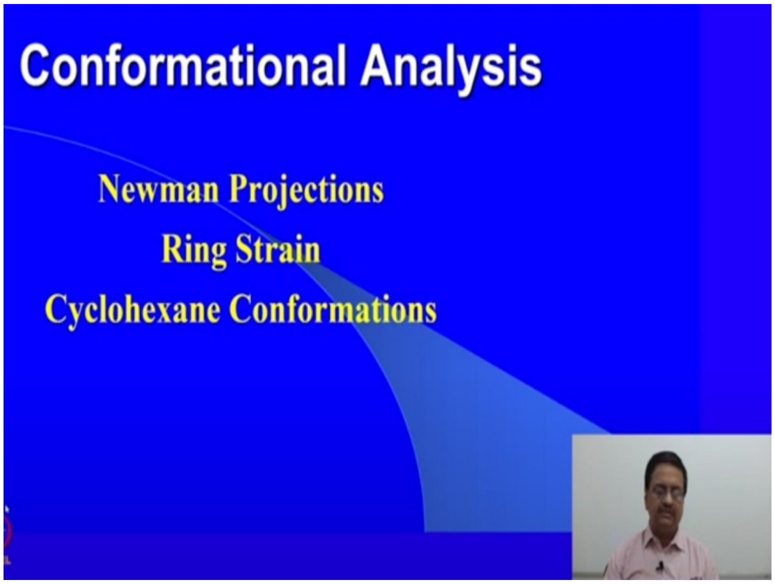

Conformational Analysis

Newman Projections

Ring Strain

Cyclohexane Conformations

In the last few lectures we were talking about the different projections, ring strain and cyclohexane conformations which we will be discuss at the later stage.

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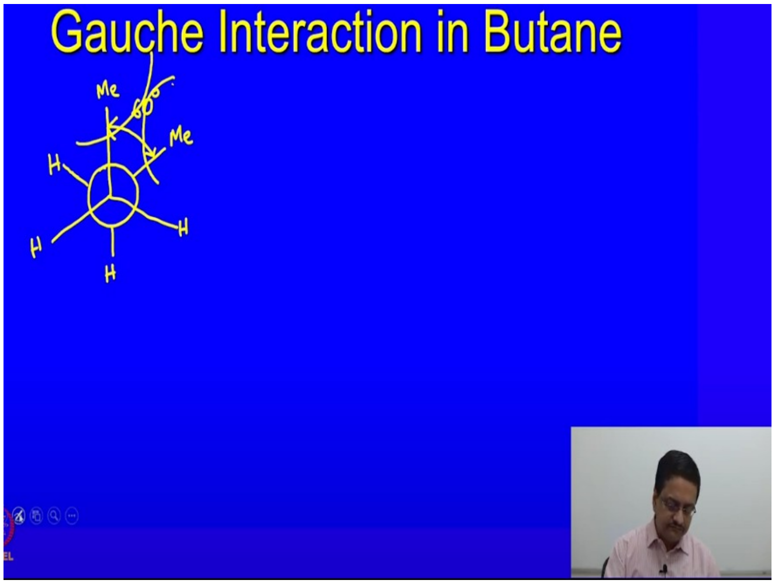

Gauche Interaction in Butane

In the last class we were talking about the conformation of n butane. And you may recall that we had drawn 4 different conformers of n butane which were fully eclipsed, Gauche, partially eclipse and anti-conformation. So let us try to now understand the various interactions present in those, different conformers. So here the title of the slides as I have indicated is Gauche interaction in butane. What does it mean?

So in case of butane, if we draw the molecule in such a way that C2 C3 is my principle axis and the groups on carbon 2 and 3 are flanked the way I am drawing then what we can see is that, In case of Gauche conformation the torsional angle between the groups in the front carbon and the back carbon is 60 degree. And when such condition appears due to the reasonably large size of methyl groups there is an interaction between the 2 methyl groups at 60 degree.

So this particular interaction is called the n butane Gauche interaction which was absent when there were 2 hydrogen atoms present at 2 carbons in case of ethane. So when you try to see this molecule in the space fill model you will see that, suppose those red one's are 2 methyl groups and those 3 methyl groups of course will have 3 hydrogen atoms in each. So in that eclipse conformation certainly they have steric strain and 0 degree torsional strain.

But then when it goes to 60 degree, steric strain is reduced but the n butane gauche interaction is present because of the bulky groups, methyl group present in that. So this particular interaction is very important in case of butane to calculate the energy difference or energy associated with these interactions for drawing potential energy curve.

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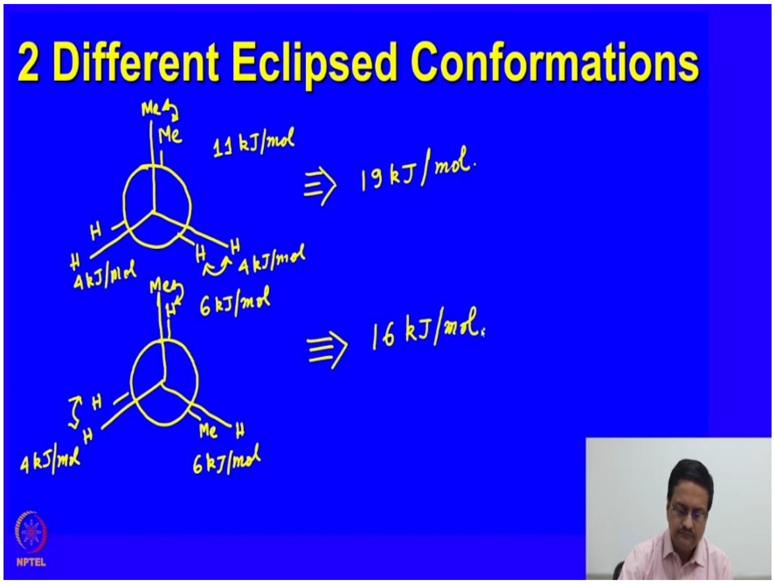

2 Different Eclipsed Conformations

As we have seen in the previous class there are 2 different eclipse conformations which are fully eclipsed and partially eclipsed conformations. So I am first drawing the fully eclipsed conformation where the methyl groups are eclipsed and hydrogens are also eclipsed. So here in this case when 2 methyl groups are eclipsed, the strain that is associated with those 2 methyl group is 11 kilojoules per mole and then the energy associated with those are as usual 4 kilojoules per mole each.

So therefore, the total energy associated with these 3 interactions is 19 kilojoules per mole. When you look for the other eclipse conformation which is not fully eclipsed conformation rather partially eclipse conformation in that the methyl is eclipsed with hydrogen and here the hydrogen is eclipsed with the methyl group. And we have 2 hydrogens which are eclipsed. So in this particular conformation the methyl hydrogen eclipsed groups have torsional strain of 6 kilojoules per mole.

We have 2 of those and we have 1 hydrogen-hydrogen eclipse conformation resulting to 4 kilojoules per mole. So the total energy associated with this conformer is 16 kilojoules per mole.

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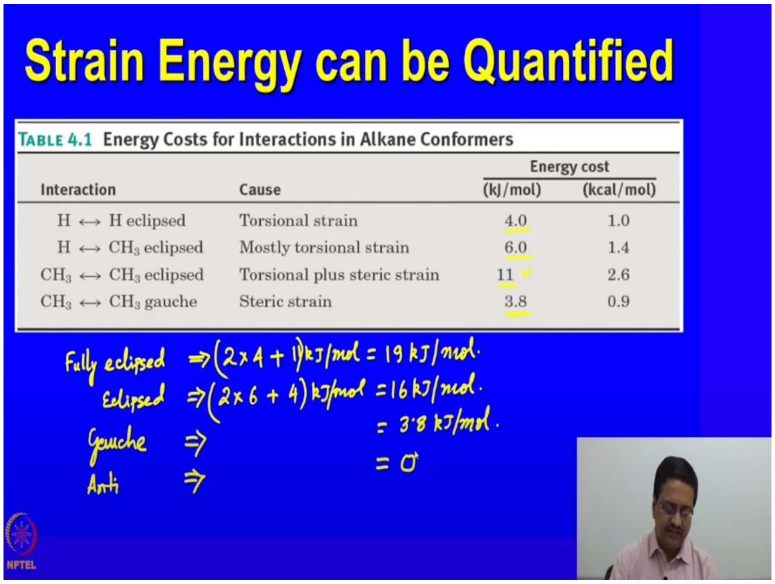

Strain Energy can be Quantified

TABLE 4.1 Energy Costs for Interactions in Alkane Conformers

Interaction	Cause	Energy cost (kJ/mol)	Energy cost (kcal/mol)
H ↔ H eclipsed	Torsional strain	4.0	1.0
H ↔ CH_3 eclipsed	Mostly torsional strain	6.0	1.4
CH_3 ↔ CH_3 eclipsed	Torsional plus steric strain	11 ✓	2.6
CH_3 ↔ CH_3 gauche	Steric strain	3.8	0.9

Fully eclipsed $\Rightarrow (2 \times 4 + 11)$ kJ/mol = 19 kJ/mol.
Eclipsed $\Rightarrow (2 \times 6 + 4)$ kJ/mol = 16 kJ/mol.
Gauche $\Rightarrow$ = 3·8 kJ/mol.
Anti $\Rightarrow$ = 0

So when you try to tabulate these numbers you can see it here that in case of hydrogen-hydrogen eclipsed 4 kilojoules per mole, in case of hydrogen and methyl it is 6 kilojoules per mole. When it is 2 methyl in eclipsed conformation it is 11 kilojoules per mole and when it is methyl and methyl just a steric strain it is 3.8 kilojoules per mole.

So if we now try to see that the fully eclipsed conformation should have 2 into 4 plus this one 11 kilojoules per mole. So it will be 19 kilojoules per mole which we have already seen. One of the partially eclipsed conformations which is this one, the first one is the fully eclipsed. Second one is the partially eclipsed conformation or just eclipsed conformation has 2 into 6 plus 4 kilojoules per mole which amounts to 16 kilojoules per mol.

And the gauche conformation should have the steric strain of methyl-methyl gauche interaction which is just 3.8 kilojoules per mole. There is no hydrogen-hydrogen steric strain in that case and the anti-conformation does not have involved in any steric or torsional strain. So we can consider that to have 0 steric or torsional strains.

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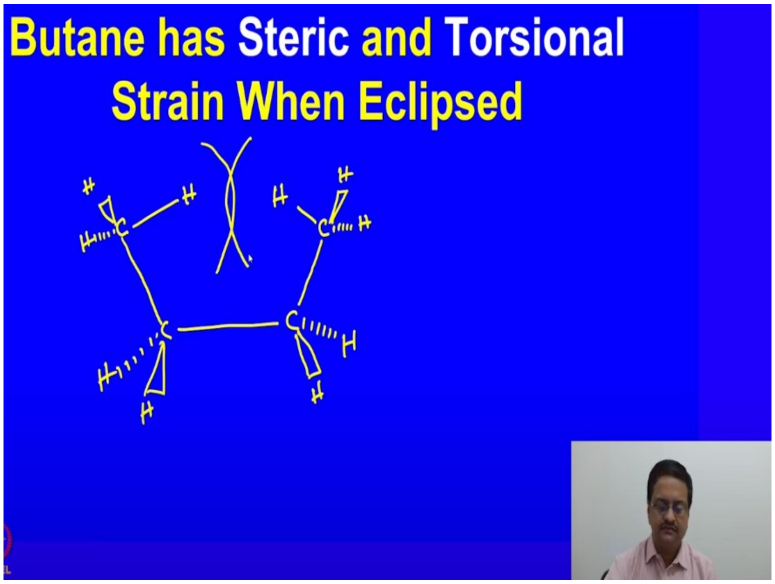

Butane has Steric and Torsional Strain When Eclipsed

So when this butane molecule is fully eclipsed what we have is the interaction associated with the methyl groups associated with the 2 carbon atoms are shown here in this way. So what we have is a steric strain when these two are eclipsed and that results in larger energy for that particular fully eclipsed conformation.

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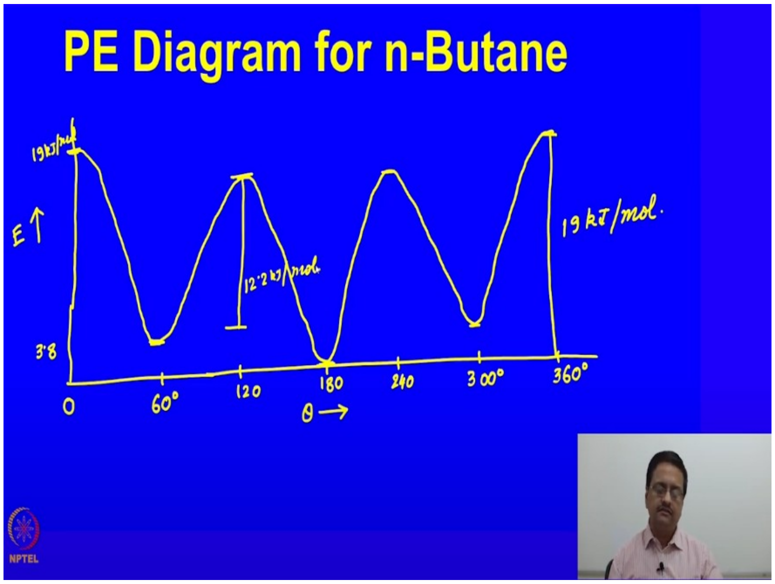

PE Diagram for n-Butane

So, when we try to draw the potential energy diagram of n butane, we need to remember those different energies for various conformations and what appears at what torsional strain. So again we draw the potential energy or the energy of the molecule in Y axis and the tortional angle theta in the X axis. When theta is 0 as we have seen that this molecules has the highest amount of destabilization amounting to 19 kilo calories per mole sorry 19 kilojoules per mole.

When you go to the conformer at 60 degree you have only the n butane gauche interaction which is 3.8. So this is 3.8 and this is 0 and this is plus 19 kilojoules per mole. Then when we go to 120 degree the conformation is we should go back and show you that the conformer should look like.

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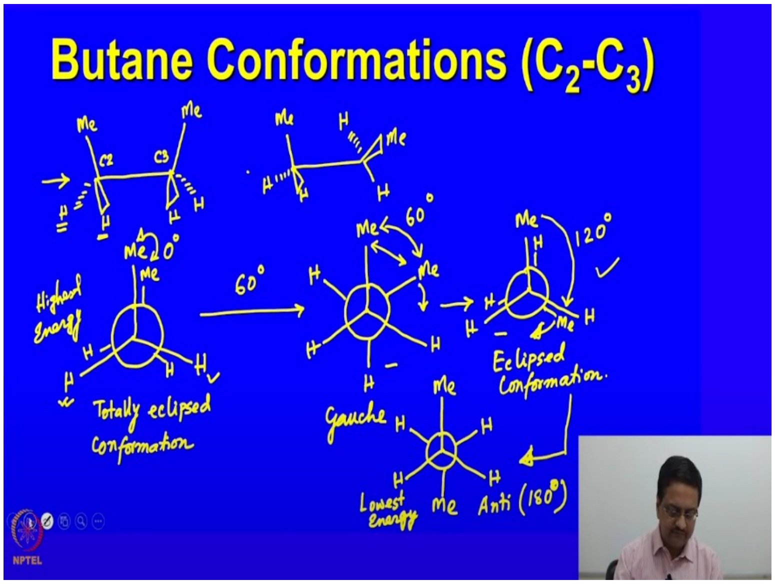

Butane Conformations (C_2-C_3)

At 120 degree the conformation will look like this where you have 2 methyl hydrogen eclipsed and 1 hydrogen-hydrogen eclipsed and the corresponding energy should be calculated accordingly. So that partially eclipse conformation has 16 kilo joules per mole. So we will draw it at a slightly lower level compared to the previous one as at this point. So when we go to 180 degree which is the anti-conformation that has the lowest energy.

So the compound or molecule exist at the lowest energy here and then you go to 240 degree you replicate the situation as same as 120 degree then when you go to 300 degree you replicate the condition of 60 degree which is somewhere here. And then when you again go to 360 degree, then it goes to 19. So the potential energy curve should look like this. So the highest energy barrier is 19 kilojoules per mole.

And the difference here is less. So this one is plus 16 and that is plus 3.8 so if you subtract it become 12.2. So this is how one can draw the potential diagram for n butane.

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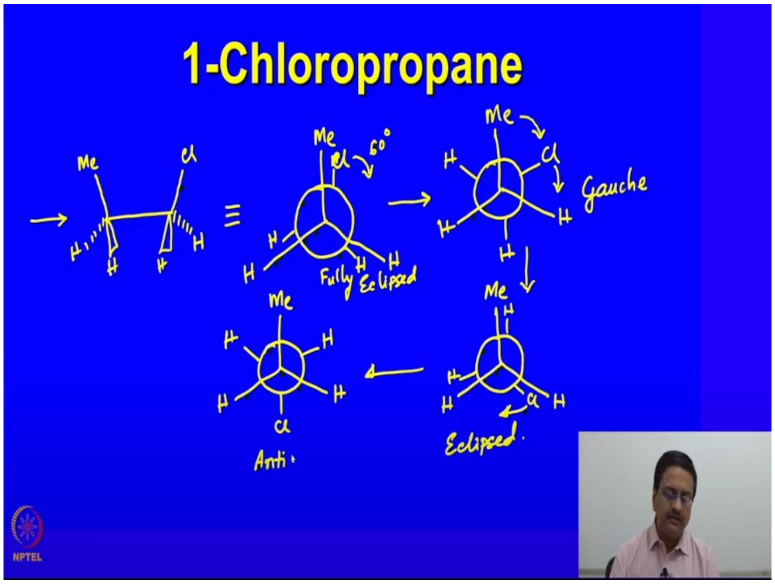

1-Chloropropane

So now let us see the example of 1 chloropropane. So here what we have is instead of butane you have 4 atoms, 3 carbons and 1, chlorine. So we can draw the molecule in this manner, methyl, the hydrogens, then you can have the chlorine instead of methyl group there and then you have the 2 hydrogens present on these carbons. So this is one chloropropane. So if you look at this molecule from this particular side and now try to draw the Newman projection it should look like this.

Here you see methyl and chlorine are eclipsed whereas the other hydrogens are eclipsed. So now if, I rotate the chlorine in the back carbon clockwise by 60 degree we would get a different conformation which is the gauche conformation here. If you continue to rotate that further what you will get is the partially eclipsed conformation like this and then you further rotate it by another 60 degree you get the corresponding anti conformation.

So this one is fully eclipsed, this is gauche, this is partially eclipse or eclipsed and this is the anti-conformation. I would like to request you to go through the previous slide and then try to draw the potential energy diagram for this particular molecule considering various interaction energies from a textbook.

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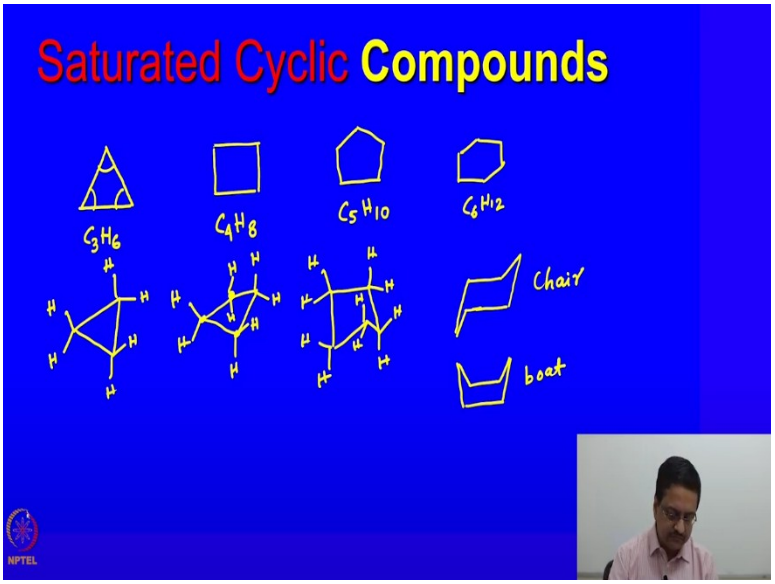

Saturated Cyclic Compounds

So with this brief introduction to the acyclic molecules and their conformations I would like to discuss now the saturated cyclic compounds and their conformations. So the first cyclic compound that one can think of is nothing but propane which has 3 carbon atoms and 6, hydrogens. What you can see is that in this particular molecule all the three carbon atoms are sp3 hybridized. But the angles are no way close to 109 degree.

So, this molecule is highly strain and hence this molecule is highly reactive and unstable. So if you try to draw this molecule as a conformation you may try to draw like that where the hydrogens are above and below, the plane of those three carbon atoms. The next one is cyclobutane. Certainly, this 4 carbon atoms in cyclobutane are not in 1 plane. So the way we can show that is the following. Assuming that 3 atoms are in 1 plane and the other atoms are slightly above the plane of those 3 atoms.

And then you have the hydrogens associated with the carbons slightly above and below the plane. The next molecule that you can have is cyclopentane. So once again here you can have 3 atoms in 1 plane and then 1 atom above the plane, the other atom below the plane and the molecule would look like this. So if you draw the hydrogen atoms this would look like that. The next molecule that we should consider is the cyclohexane which we draw just like this indicating that the hydrogens are present.

So the formula is C6H12 and we will discuss the conformation of this molecule in detail in next few minutes. So this molecule has a conformation which is like this which is called a chair conformation and the other conformer is called a boat conformation which is this one. There are, other intermediate conformation which we discuss very soon.

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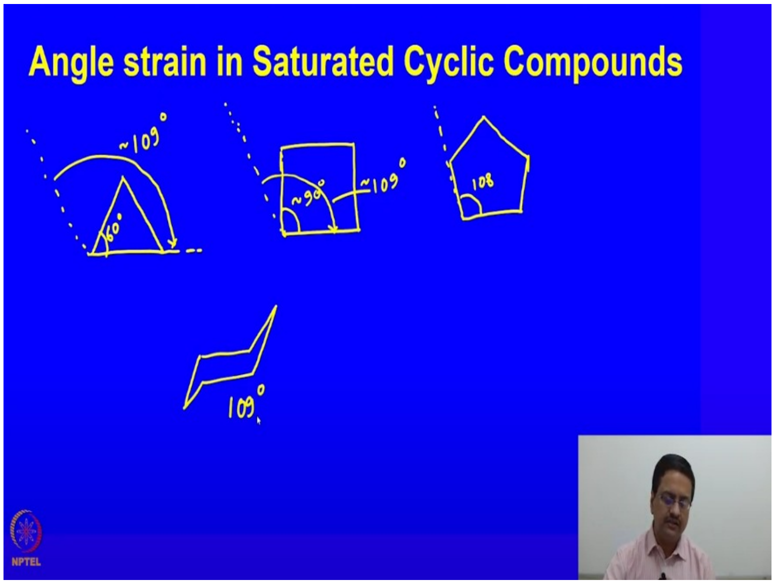

Angle strain in Saturated Cyclic Compounds

So when you see these various small organic cyclic compound you can easily understand that this molecules have significant amount of angle strain. In case of cyclopropane, the angle here is 60 degree but it should have been ideally a tetrahedral angle of 109 degree. So that is why this molecule is highly strained. So the next molecule that we had drawn in the previous slide is cyclobutane. This angle is closed to 90 degree but ideally again this being a sp3 carbon this angle ideally should have been 109 degree.

So this has a slightly lesser strain compare to cyclopropane. And in case of cyclopentane that angle is about 108 degree which is close to 109 and hence cyclopentane is not that unstable like others in this group. In case of cyclohexane the way we draw the conformers always the angles are 109 degree. So there is no angle strain in case of cyclohexane molecule.

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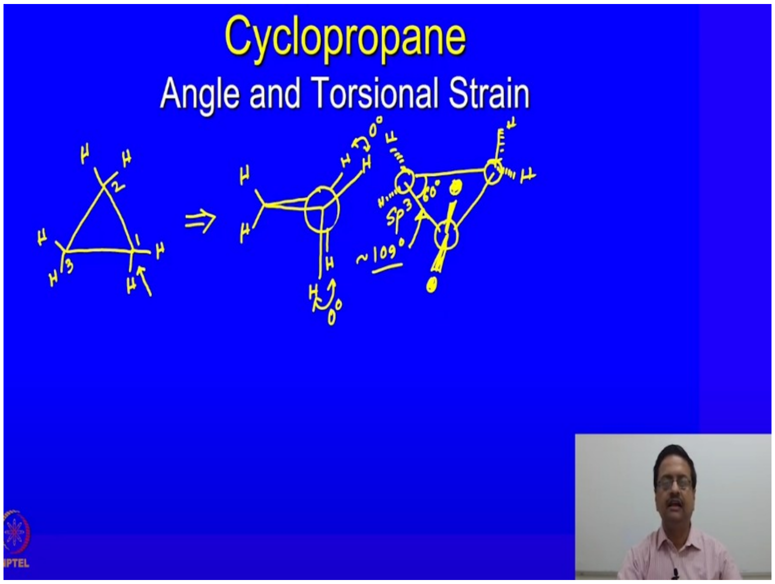

Cyclopropane

Angle and Torsional Strain

So now let us see the angle and torsional strain that is observed in case of cyclopropane. So what we know about cyclopropane is that the molecule has 3 carbon atoms and those 3 carbon atoms lie in 1 plane and each of them contains 1, hydrogen making it cyclopropane. So if I try to draw this molecule in such a way that we look through this C-C bond and draw the molecule in Newman projection.

So then it would look like this. On the front carbon we will have 2 hydrogens and the on the back carbon as well we should have 2 hydrogens in the eclipse conformation. And this front carbon through the carbon 3 is connected to the back carbon like this and this has 2 hydrogens. So here what we see is that the molecule is in eclipse conformation and all the hydrogens are eclipsed and there is enormous amount of torsional strain because of 0 degree angle or 0 degree dihedral angle between the hydrogen atoms.

So if you try to draw the molecule in a way that we are seeing from the side of 1 carbon atom. The other 2 carbon atoms are behind. What I am trying to draw is a ball and stick model of this particular compound and I am trying to show it with Wedges or rather spheres saying that this are hydrogens for this there will be hydrogens at the back and here there will be hydrogens at the back. So these molecules has very high angle strain because you see this bond angle is 60 degree which is very far deviated from the ideal value for sp3 carbon to be 109 degree.

So instead of 109 degree the deviation is large. So you have a large angle strain in the molecule and also these hydrogens are in eclipsed condition so the molecule has an additional torsional strain as well. And therefore this molecule is highly unstable.

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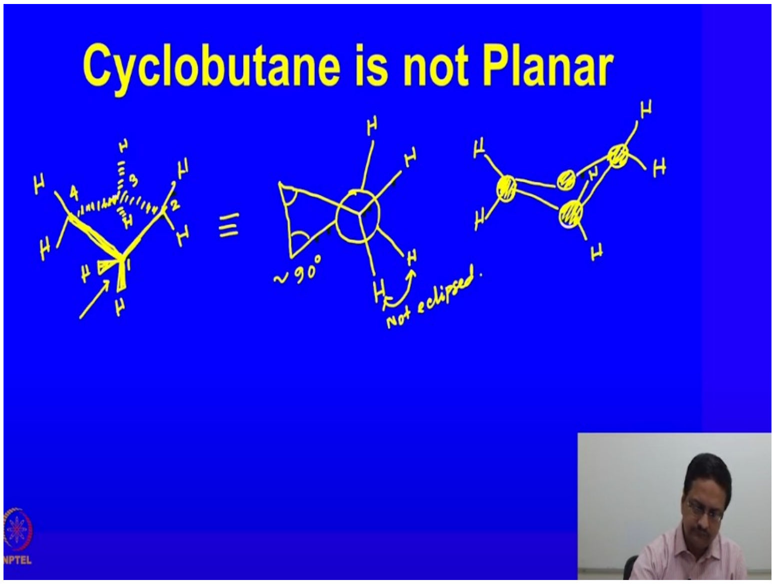

Cyclobutane is not Planar

So here all the dihedral angle that we have seen is 0 degree. Now let us look at cyclobutane. As we can understand or we all know that cyclobutane is not a planar molecule. So the way I am drawing is to show that the 2 carbon atoms which are probably on the plane and then there is 1 carbon atom which is above the plane of the presentation or above the plane of the board and the other carbon atom is behind the plane of the board like that.

So we have 2 hydrogen atoms on this 2 carbon atoms which look like that. And then the other 2 hydrogen on these carbons are pointed towards us. And the hydrogens on the back carbon are pointed backwards. So, now if we try to draw the corresponding Newman projection of this molecule by looking through this bond. Let us number it as 1, 2, 3 and 4. So the Newman projection of this molecule will look like this. So here the hydrogen atoms are not eclipsed.

And not actually in the gauche conformation that it is about 60 degree. So it is not 60 degree but it is not fully eclipsed. So it has a less amount of torsional strain compared to cyclopropane. And due to presence of 4 carbon atoms these angles are close to 90 degree or may be slightly more than 90 degree. And as a result, it has less angular strength. So if can try to draw this molecule using this ball and stick model one can think of drawing it like this. So then you have the hydrogen atoms like that.

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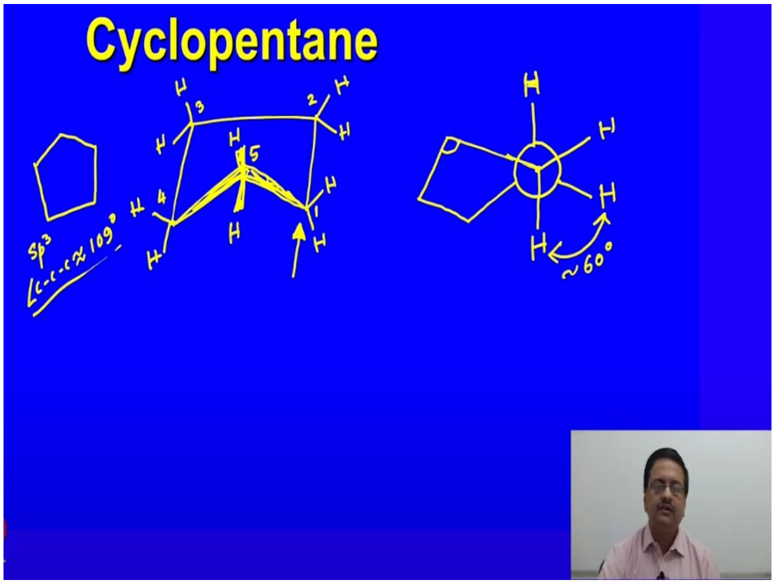

Cyclopentane

Now let us see the conformation of cyclopentane. Although in the text book we may be writing the molecule as a planar molecule just like this, the molecule is not a planar molecule because we have 5 carbon atoms which are all sp3 hybridised carbon atoms; sp3 bonded carbon atoms and all are trying to become tetrahedral maintain a CCC angle close to 109 degree. Therefore this molecule is not a planar molecule.

So when we try to draw it with the corresponding 3 dimensional view keeping in mind, the molecule should like this. So 2 hydrogen atoms on the back carbons are pointed backwards, 2 hydrogens on these carbons are on the planar projection and again 2 hydrogens projected towards us on this carbon which is above the plane of projection. So now if we try to draw this molecule in the Newman projection by viewing through this C-C bond which I try to name it as 1, 2, 3, 4 and 5.

What do you see is that the back carbon is number to 2 and the front carbon is number 1. So the front carbon has 1 hydrogen down and 1 hydrogen here and then this gets connected to the carbon number 5 and then that gets connected to carbon number 4 and that carbon number 4 is in turn connected to carbon number 3 and then it is connected to carbon number 2. So what we see is that it attains a gauche type of conformation which is not eclipsing bond. So the eclipsing torsional strain released it is closed to about 60 degree and it is like a gauche conformation and we have all hydrogens at a torsional angle of 60 degree.

So the torsional strain is released. And there is a little angle strain and hence cyclopentane is more, staple than cyclopropane and cyclobutane. So we will continue our discussion in the next lecture from here.