Introductory Organic Chemistry

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Lecture – 06

Alkanes & Cycloalkanes Part - 1

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Hi. Throughout our first few lectures we are going to stress upon the structural properties of organic compounds because once we understand the structure of compounds, we can then proceed to the reactivity of these compounds because structure always governs the reactivity of molecules.

So, today we are going to study the structural properties of Alkanes and Cycloalkanes. So, in this chapter we will go over the structure of alkanes, cycloalkanes, their conformational analysis and then we will proceed to the physical properties of alkanes and cycloalkanes.

So, alkanes are hydrocarbons meaning they only contain two elements, carbons and hydrogens. Very often you will hear that term called as aliphatic hydrocarbon for alkanes because aliphatic comes from the Greek word ‘aleiphar’, meaning animal fat or plant oils and if you see the higher alkanes you will see that their properties are very similar to that of animal fats or plant oils. So, aliphatic hydrocarbons meaning they contain carbon and hydrogen and they have properties similar to that of animal fats and plant oils. We also know that alkanes are saturated hydrocarbons meaning they only contain carbon-carbon single bonds in them; there is no pi bond between two carbon atoms.

In the last class we looked at the structure of methane and we look how carbon forms sp3 hybridization; it has four of these sp3 hybridized orbitals which then overlap with the 1s orbital of each hydrogen atom and you have this tetrahedral geometry that results because of it, with the bond angle of 109.5 degrees.

Next alkanes in the series are ethane, propane, butane and so on and most of them will have similar properties in the sense that the hybridization will be sp3 for the carbon. The bond angle may change a little bit from 109.5 degrees, but not much. But, before we go into the details of their structural properties, first let us look at how we represent them on paper.

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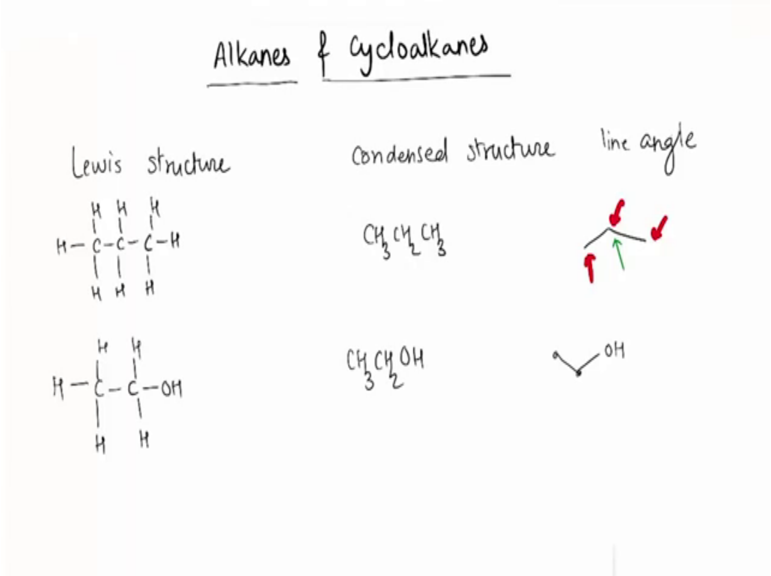

Alkanes & Cycloalkanes

Lewis structure

Condensed structure

line angle

$CH_3CH_2CH_3$

CH_3CH_2OH

So, now, we will look at line angle formula which is very often used by chemist to represent organic molecules on paper. Remember the Lewis structure of propane? If I want to draw Lewis structure of propane it will look somewhat like this wherein carbon is forming bonds with all the hydrogens, right and you may also show electron dot structures so you may also show the electrons in them.

Now, if I want to write the condensed structure of the same propane molecule I will represent it like $CH_3CH_2CH_3$ wherein I don't draw the individual bonds, but it will look looks as a condensed structure. And the most common method to represent propane would be using a line angle structure which is something like this; wherein each of this vertex represents the carbon. Vertex or the end of the line will represent the carbon that is present; we do not represent the hydrogens present in the molecule. Very often you assume that those many number of hydrogens are present as per the carbon that is forming the bonds.

So, for example, in this case the middle carbon here is forming two bonds with other two carbons. So, it will have two hydrogens on top of it whereas, the terminal carbons are only forming one bond so, they will have three hydrogens attached to them. So, we assume that the number of hydrogens are present in order to fulfill the valency of each carbon. Let us look at one more structure.

Here is, for example, the structure of ethanol, okay. Now, ethanol as you can see, really does not look like what we represent it on papers. So, if I want to draw the structure of ethanol on paper it will look or a Lewis structure of ethanol it will look somewhat like this, right. This is not how the molecule looks like. In fact, if you look at the molecule it has particular geometry such that there is a bond angle between carbon – carbon and oxygen that will always be there.

In order to draw the condensed structure, I will write it as CH_3CH_2OH right so, condensing it together and in order to draw the line angle structure we will represent it something like this when in each of these vertexes again the carbon and there is an OH attached to one of the carbons. So, if we go on writing now the Lewis structure, the condensed structure and the line angle formula for the first ten alkanes it would look something like this.

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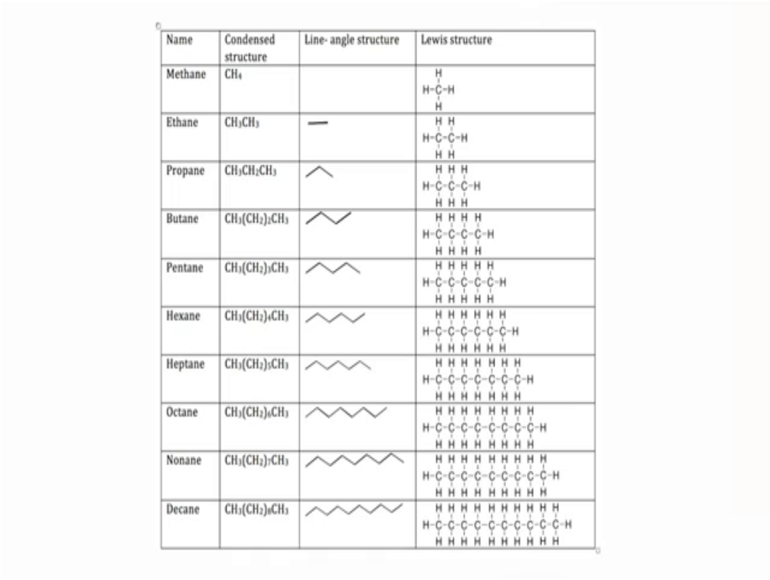

Name	Condensed structure	Line- angle structure	Lewis structure
Methane	CH_4		H H-C-H H
Ethane	CH_3CH_3		H H H-C-C-H H H
Propane	$CH_3CH_2CH_3$		H H H H-C-C-C-H H H H
Butane	$CH_3(CH_2)_2CH_3$		H H H H H-C-C-C-C-H H H H H
Pentane	$CH_3(CH_2)_3CH_3$		H H H H H H-C-C-C-C-C-H H H H H H
Hexane	$CH_3(CH_2)_4CH_3$		H H H H H H H-C-C-C-C-C-C-H H H H H H H
Heptane	$CH_3(CH_2)_5CH_3$		H H H H H H H H-C-C-C-C-C-C-C-H H H H H H H H
Octane	$CH_3(CH_2)_6CH_3$		H H H H H H H H H-C-C-C-C-C-C-C-C-H H H H H H H H H
Nonane	$CH_3(CH_2)_7CH_3$		H H H H H H H H H H-C-C-C-C-C-C-C-C-C-H H H H H H H H H H
Decane	$CH_3(CH_2)_8CH_3$		H H H H H H H H H H H-C-C-C-C-C-C-C-C-C-C-H H H H H H H H H H H

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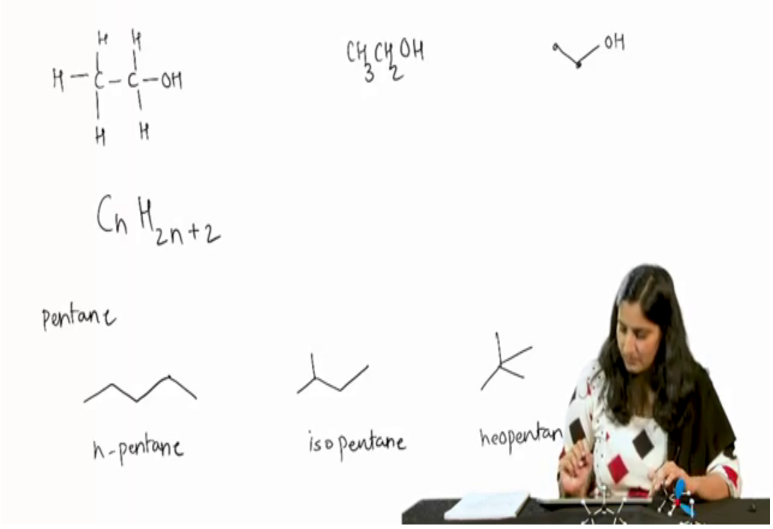

Alkanes have a general formula of C_nH_{2n+2} meaning for every n number of carbons there is 2n plus 2 number of hydrogens present in the molecule. In the last class we also looked at isomerism which talked about having the same molecular formula, but different structural formulas. So, we looked at butane and isobutane for example, in the last class and as you go on increasing the number of carbons the number of possible constitutional isomers also go on increasing tremendously.

So, for example, here I have pentane and pentane will have; here I have pentane, so, pentane has five carbons and pentane will have the following constitutional isomers. So, this is n-pentane, next we have isopentane and then we have neopentane, okay. So, the line angle formulas for all the isomers of pentane look like this.

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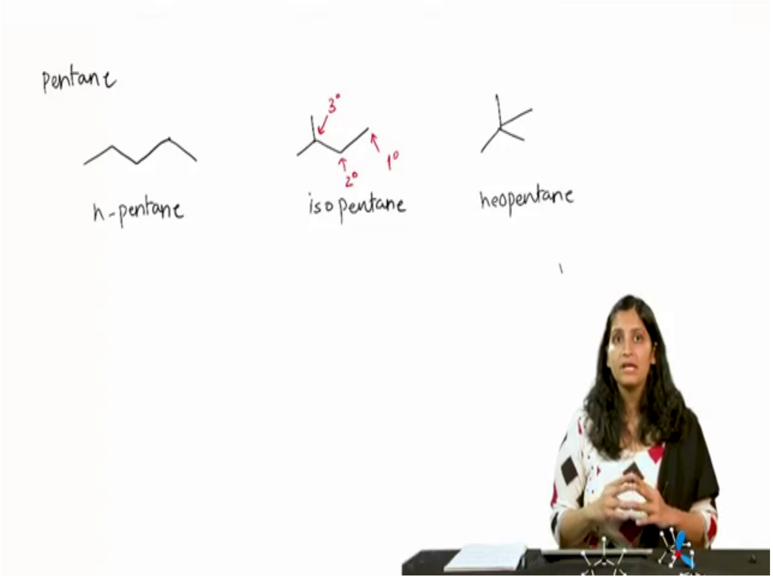

Now, you may think that for butane which had four carbons the number of isomers were two; as we go to pentane the number of isomers get to three. So, maybe they will just go on increasing by the number of carbons, but if you really count the possible number of isomers that are possible as we go on increasing the carbons I have a few numbers here and you can look at them that for methane that are zero constitutional isomers; as we go to pentane so, for five carbons there are three structural isomers or constitutional isomers as we call them.

As we go on increasing the number of carbons further, so, let's go to 10 carbons; now 10 carbons will have 75 constitutional isomers and if I increase the number to 15 the number of constitutional isomers goes to around 4000. If I increase the number to 25 carbons the number of constitutional isomers that a carbon compound can really have are close to 37 million. So, you can imagine that as we go on increasing the number of carbons even for a small number of carbons which is 25 you can have up to 37 million compounds. And this is one of the reasons that carbon molecules can be found everywhere and we are able to get so many molecules that are just arising from the carbon and hydrogen itself.

Very often you will also hear the term called as primary carbon, a secondary carbon, a tertiary and a quaternary carbon. So, what are these? So, chemists use these terminologies to represent the number of bonds each carbon is forming. So, for example, here I have isopentane and if you look at this particular terminal carbon, it is forming bonds with only one carbon that is next to it. So, it becomes a primary carbon, okay. The carbon next to it is forming bonds with two other carbons, so, what you have here is a secondary carbon and the carbon next to it is forming bonds with three other carbons. So, that becomes a tertiary carbon.

Very often you will see that reactivity depends on whether a particular atom in our case carbon is primary, secondary or tertiary. So, when we go over a few reactions henceforth we will first judge if the compound has a carbon that is primary or secondary and then decide how it would react in a chemical reaction. Just like us when we like our name to be unique chemists also wanted all the compounds to have a very unique name such that the structure and the properties of that compound could be determined just by looking at the name of the compound and chemists have used a set of rules governed by IUPAC which is the International Union of Pure and Applied Chemistry to design a set of rules in order to describe molecules.

We are going to go over a tutorial that solely goes over IUPAC rules and nomenclature for alkanes, alkenes and alkynes and alkyl halides in this particular course. So, if you want to go over the details of nomenclature you can refer to the tutorial. For now, I have given you the names of the first few alkanes and their structures in this table. If you look at the table, each of these names has a prefix and a suffix. So, prefix is like your name your given name which is representing you whereas, suffix belongs to the family name, so, like your surname.

So, all the alkanes have the surname or the suffix as ‘ane’ indicating that they belong to the class of alkanes and where as prefix can be meth, eth, prop and so on; combining it together you get methane, ethane and propane and so on. Representing a given name and family name meaning a prefix and a suffix will complete the name of the particular alkane. So, we will cover a detailed nomenclature of alkanes, substituted alkanes, cycloalkanes and bicyclo compounds in this week’s tutorial.

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So, structural formulas are good to represent things on paper, but they hardly tell us how the molecule really is in a 3D space. And it is very important for us to understand the 3D nature of molecules to determine the reactivity of these molecules. So, just now we looked at the structural formula of ethanol, but it hardly represent the structure which is representing of the bond angles, representing of the lone pairs present, representing of the different bond lengths that are between the atoms.

So, if you want to really get a feel of how a compound can react it is very important to know what is the 3D structure of the molecule. Not only the 3D structure, but you should also be able to predict what are the bond angles, what are the bond lengths and also how is the electron density distributed between the bonds. So, for example, in this case I have ethanol. So, right now what I have is a bond between oxygen and hydrogen and it is a polar covalent bond so, which means that most of the electron density of this bond is with the oxygen and not with the hydrogen.

So, as a result of which when ethanol reacts with a base this particular hydrogen will be easily removed because it does not hold an equal share in the bond electron density. So, as you can see imagining the 3D structure, imagining the bond lengths and the electron density between the bonds will allow us to gaze the reactivity of a particular molecule. So, hence forth in the course we are going to get a feel of the structure first and then proceed to the reactivity, but just imagining the 3D structure is also not enough. We also need to know how these bonds rotate.

So, for example, right now I am rotating the carbon – carbon bond such that it is rotating and giving rise to different conformations. So, we will go over conformational analysis which talks about these conformations that arise as the bonds or single bonds rotate around each other.

Strain is a key concept in organic chemistry. It is representative of the energy stored in the molecule because of distortion. Soon we will go over three types of strains present; one is a torsional strain, angle strain and steric strain and all of these three types of strains play a role in which the molecule reacts.

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Conformational analysis

'Strain'

Strain in general refers to a molecule not being in its most stable form or optimal form. Anytime we change the structure or we input some disturbance into the system we give rise to the strain which the molecule has to experience. So, for example, if this is the most stable form of the molecule and if I change and rotate the structure, there might be some strain that this molecule is experiencing right now.

Strain also represents the energy stored in the molecule. So, if there is enough energy. So, you can imagine really windy situation if there is enough energy then the tree branches gonna go back and forth because there is enough energy for these inter-convergence to happen.

Now, in the chemical system the inter-convergence of various conformations happen because there is enough, either temperature that is the thermal conditions or there are collisions that these molecules are experiencing which will make them rotate and give rise to various inter-convergence of the state.

You will also see that some structures are permanently strained. So, just like that compressed spring if I keep that spring completely compressed all the time there will be a permanent strain into that system. Just like that some of the molecules you will see are permanently strained and they are very eager to release this energy in reaction. So, we see that these molecules have a higher reactivity, they will undergo reactions much quickly than some other molecules because they want to release the energy that is stored inside them.

So, now let us look at strains in alkanes. So, I have an ethane molecule and it has two carbons and six carbon-hydrogen bonds. As you can see, as I change the conformation meaning as I change the position and rotate this front carbon keeping the back carbon the same, if I rotate it clockwise or anticlockwise I give rise to various conformations.

Now, conformation refers to the 3D arrangement that arises because order of rotation of this carbon – carbon single, okay. So, anytime I rotate I give rise to a different conformation of this ethane molecule. So, let us look at the conformations of ethane now. This particular conformation in my hand is called as eclipse conformation. Eclipse conformation refers to the overlap between the bonds. So, for examples a carbon – hydrogen bond of the first carbon is overlapping with the carbon – hydrogen bond of the second carbon and you kind of have them eclipsed with each other. So, this is an eclipsed conformation.

Now, if I rotate this front carbon such that keeping the back carbon the same, what do I give rise to? I give rise to a different conformation such that now these bonds are farthest apart from each other such that the bond angle between this and this is now 60 degrees. So, this particular conformation is called as a staggered conformation. Now, if I want to represent it on paper what I used is called as a Newman projection, okay.

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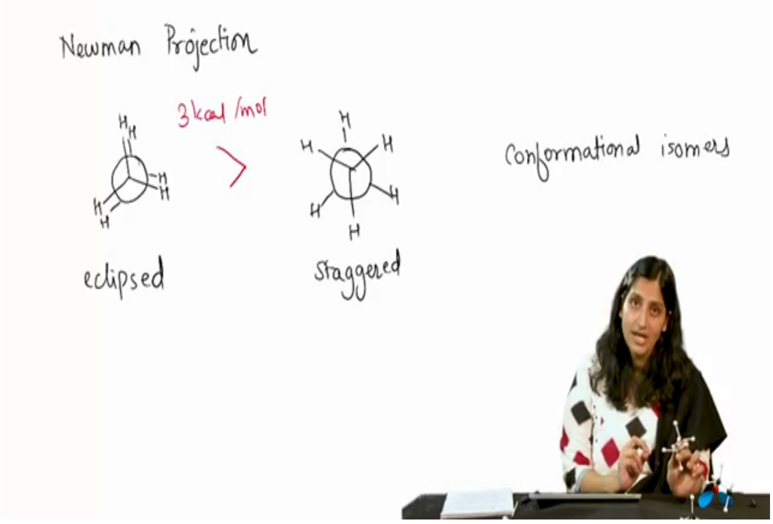

So, Newman projections represent a molecule such that you are able to represent these conformations. So, now, if I want to draw this particular eclipsed conformation of ethane, if you really look at it, the front carbon has three bonds, 3 carbon–hydrogen bonds and the black carbon also has 3 carbon–hydrogen bonds. In order to show that they are eclipsed with each other I am going to show them very close to the first bond, okay. Now, ideally it is very difficult to represent it on paper such that they are completely overlapping with each other. So, this is my eclipsed conformation.

And now if I want to represent the staggered conformation, remember I have kept the back carbon the same, right and I move the front carbon such that it now represents this structure. okay. So, then you have the staggered conformation which is in this state. Since I can rotate and interconvert the staggered to eclipse and eclipse back to staggered by just rotating a carbon – carbon single bond, these two forms, the eclipsed form and staggered form are called as conformational isomers of each other. So, these two are conformational isomers.

So, if we take an ethane molecule this bond is kind of continuously rotating or rather spinning around each other such that the molecule is constantly going on between the eclipsed and the staggered form as represented. It is easier to discuss the energy differences between the eclipsed and staggered form in terms of the dihedral angle. So, for example, right now the dihedral angle between the two planes is 0, okay; meaning that it is all in the eclipsed fashion.

Now, if I slowly rotate this back carbon, the dihedral angle between this plane and this plane will get to 60 degrees. Again, if I go on rotating I will go back to again the dihedral angle being 0 and an again 60 and so on. So, it is easier to represent the conformations or the conformational isomers with the help of the dihedral angle that is present in between them. In principle, there are infinite conformations present as I slowly change this dihedral angle slowly. So, we directly change it from 0 to 60. You need not change it from 0 to 60; slowly changing will give rise to really infinite number of conformations that are possible in this case.

So, now, let us look at the energy difference. As you can imagine the eclipsed conformation is a little bit strained, okay. We will go over the reason why it is strained later in this talk, but remember that eclipse conformation is around 3 kilo calories more in energy than that of the staggered form. The staggered form is a little more stable because the carbon – hydrogen bonds are farthest apart from each other, okay. In this case the 2 carbon – hydrogen bonds are overlapping.

So, you can say that approximately a carbon hydrogen bond eclipsing with other carbon – hydrogen bond, the energy for this interaction is about 1 kilo calories per mole and together I have three of these bonds. So, I have 3 kilo calories difference between the eclipsed and the staggered conformation, okay. So, I will write that this eclipsed one is around 3 kilo calories per mole more than the staggered form and this particular strain or this particular energy is also called as torsional strain. So, what the eclipsed conformation is undergoing is a torsional strain because of the eclipsing of the carbon – hydrogen bonds.

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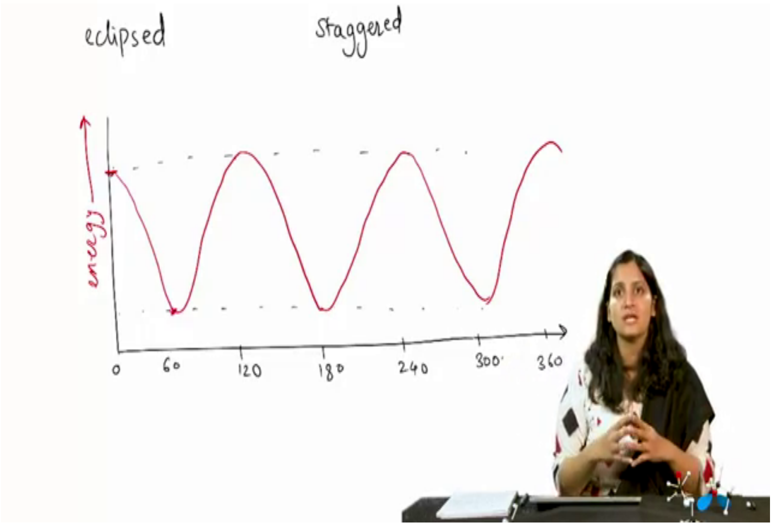

Okay, so now if I want to plot the graph such that this particular carbon – hydrogen bond is rotated such that it completes one complete rotation; okay so, now, this is a modified ethane what I have done is I have just replaced the 2 hydrogens with two colors, so that it is easier to visualize.

Now, the bond angle currently between these two carbon – hydrogen bonds is 0 degrees, it is eclipsed. So, it is 3 kilo calories more in energy. As I slowly rotate this back, hydrogen which is green in color, the dihedral angle between the two carbon hydrogens, the red and the green one, is now 60 degrees. At 60 degrees the molecule is in a staggered conformation which is lower in energy by 3 kilocalories. So, I will draw this to be at 60 degrees, the energy is going to go down.

As I further move this such that these two carbon – hydrogen bonds have a dihedral angle of 120 degrees. At 120 degrees we have gotten back to the eclipsed conformation. So, it will be again higher in energy, okay. So, if I go to 180 degrees we are back to staggered they are farthest apart from each other. So, this is again lower. So, at 180 degrees the energy will go down.

Again the dihedral angle between these two planes is now 240 degrees. So, at 240 degrees we have a higher energy because this is again eclipsed conformation and as I proceed to 300 degrees, it is staggered. So, I will again make it go down in energy. Back to 360 degrees' rotation, we are back to the eclipsed conformation.

So, as you can see that every time I rotate the energy that the molecule has to go through or the strain that the molecule has to go through, which is just two different words for the same concept, it goes on increasing and decreasing based on the dihedral angle between the two bonds.

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So, what could be the origin of the torsional strain? This particular debate has been going on for a lot of decades and chemists are still trying to figure out what is the exact origin of the torsional strain. At first it was believed that the strain results because of the repulsion between, let’s say, these two hydrogen nucleis; in the eclipsed fashion they are very close to each other. So, there is a repulsion between these two hydrogen nucleis.

There was another theory which talked about that the strain results because of repulsion between the electron density in the bonds. So, for example, these two carbon – hydrogen bonds will have repulsion between them because there are electrons present and they will repel each other. However, the calculations or the computational models suggest something different and for this we need to think about the molecular orbital theory again.

So, the theoretical calculation suggest that the energy difference is not because of the destabilization that occurs because of the eclipsed fashion, but it is rather because of the stabilization that can be achieved in the staggered conformation. So, what is this stabilization? The stabilization in the staggered conformation arises because of a donor acceptor kind of relationship. So, in order to understand this, we need to go back to the molecular orbital theory.

If you remember the bonding molecular orbital for this particular carbon hydrogen bond will go in this direction, in the direction of the bond whereas, the anti-bonding molecular orbital will go in the opposite direction, okay. So, if you really see an overlap can happen between the bonding molecular orbital of the back carbon – hydrogen bond with the anti-bonding molecular orbital of the front carbon – hydrogen bond. So, because of this in the staggered conformation, there is a partial overlap happening such that the electron density from this bond kind of gets transferred towards the anti-bonding molecular orbital of this particular bond.

Now, remember we are not actually transferring the electrons because that would result in the breaking of the bonds. We are not actually transferring the electrons, but we are kind of overlapping these two orbitals which results in stabilization. So, the energy difference between the eclipsed and the staggered conformation arises because you have an overlap between the bonding molecular orbital and anti-bonding molecular orbital that happens in the staggered conformation. As I quickly move to the eclipsed conformation, now both the anti-bonding molecular orbitals are in the same direction, there is no longer any overlap possible. So, this overlap is lost as we move to the eclipsed conformation.

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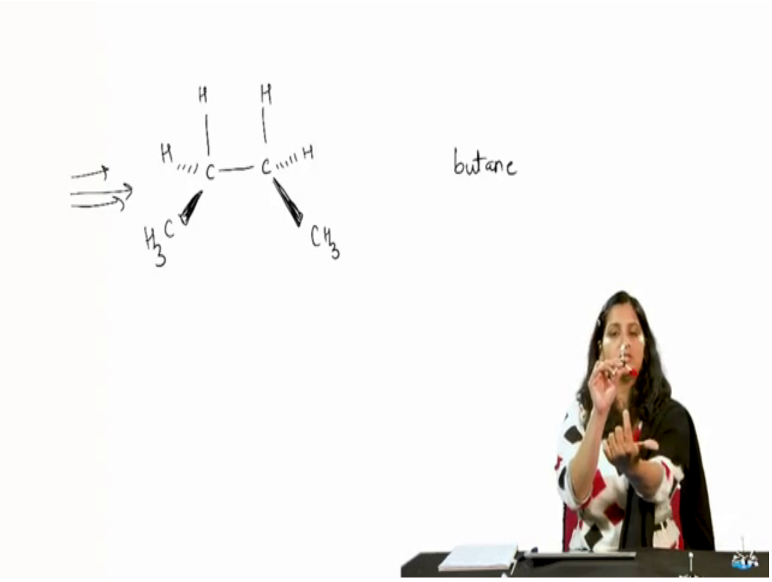

So, now let us look at the conformational analysis of butane. What I am going to do is; so, let’s imagine that this is a butane molecule and these two are the methyl groups. So, $CH_3CH_2CH_2CH_3$, so, that is a butane molecule and we are going to look at the conformations as we rotate the bond between C 2 and C 3. So, carbon number 2 and 3 as they rotate the bond between them what kind of conformations arise? Okay.

So, I have drawn a particular representation of butane here in order to understand this what you can imagine is that the wedges are such that the bonds are coming towards you and the dashes are such that the bonds are going away from you. So, in your case the two bonds between the carbon and the methyl groups are coming towards you and the dashed version of the bonds are the bonds that are going away from you whereas, these four bonds are in the plane of the paper, okay.

So, now if I am visualizing this particular molecule such that I am looking at it from this point, from this angle such that let’s imagine that you are looking at it from this side how would the molecule look to you?

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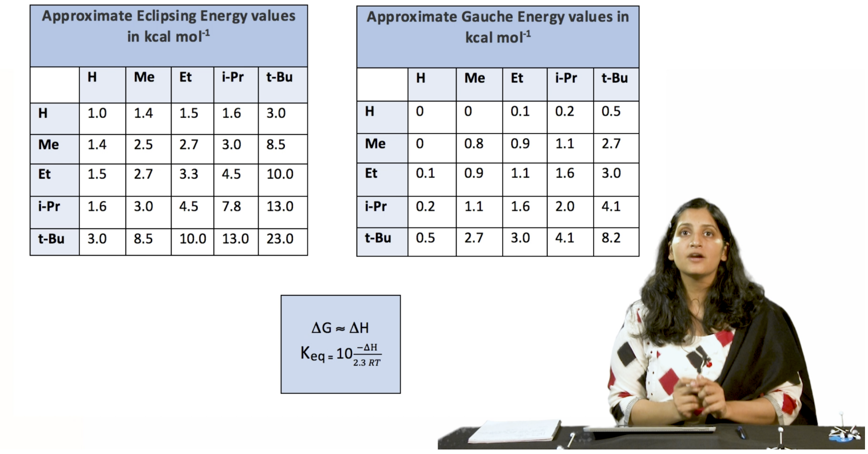

Approximate Eclipsing Energy values in kcal mol^{-1}

	H	Me	Et	i-Pr	t-Bu
H	1.0	1.4	1.5	1.6	3.0
Me	1.4	2.5	2.7	3.0	8.5
Et	1.5	2.7	3.3	4.5	10.0
i-Pr	1.6	3.0	4.5	7.8	13.0
t-Bu	3.0	8.5	10.0	13.0	23.0

Approximate Gauche Energy values in kcal mol^{-1}

	H	Me	Et	i-Pr	t-Bu
H	0	0	0.1	0.2	0.5
Me	0	0.8	0.9	1.1	2.7
Et	0.1	0.9	1.1	1.6	3.0
i-Pr	0.2	1.1	1.6	2.0	4.1
t-Bu	0.5	2.7	3.0	4.1	8.2

$$\Delta G \approx \Delta H$$
$$K_{eq} = 10^{\frac{-\Delta H}{2.3\,RT}}$$

So, I am imagining that you are looking at it like this. So, if I am looking at from this side I have. Okay, so the front carbon has the bond such that the carbon and hydrogen bonds are there and then there is a carbon methyl bond. Now, if I want to represent the back carbon I will also draw it which will be like this, okay.

Now, remember we talked about hydrogen – hydrogen eclipsing which results about 1 kilo calories per mole of torsional strain in the molecule. Remember, when two methyls are eclipsing with each other the strain is going to be even more and it is approximately 2.5 kilo calories per mole. So, in order to refer to the eclipsing interaction of various groups here is a table and you can refer to it and figure out what is the torsional strain that results because let us say when methyl-methyl kind of overlap with each other versus when a methyl and hydrogen eclipse with each. So, the energies are going to be different and you can refer to this particular table.

For now, we are going to assume that the methyl methyl eclipsing will be 2.5 kilo calories, each of these eclipsing interactions will be approximately 1-1 kilo calories per mole. So, total right now the energy of this particular molecule or the strain that this particular molecule is experiencing will be 2.5 plus 2 which is close to 4.5 kilo calories per mole. So, this particular conformation will be highest in energy because I have a methyl-methyl eclipsing with each other.

So, now, what I have here is the representation of this particular eclipsed conformation of butane and I am going to slowly increase the angle. So, right now the dihedral angle between these two methyls is 0. I am going to slowly increase such that the dihedral angle becomes 60 degrees.

So, what I am going to do is, I am going to increase it such that the dihedral angle becomes 60. We will keep the front carbon the same and we will move the back carbon ok. So, this was at 0 degrees, this is at 60 degrees. If I go on drawing what I will have is; okay so, this is at 60 degrees. Now, let us make the dihedral angle to be 120 degrees with respect to each other.

So, at 120 degrees again we have gotten back to the eclipsed conformation. If I move it further I give rise to 180 degrees, okay. So, this is 120, 180. Let us draw, at 240 degrees what is the case? So, then I keep the front carbon the same I will move this back carbon here to go to 240 degrees, then we have 300 degrees. Keep the front carbon the same I will move the back carbon such that it goes here and then we are back to 360 degrees wherein we get back to our original conformation where we started from. So, these are our conformations as we go from 0 degrees slowly rotating and getting back to 360 degrees, okay.

Now, let us try to analyze the energies of these molecules. As we know that every kind of eclipsed conformation will have a higher energy because of the torsional strain present in the molecule. So, I am going to circle my eclipsed conformations. First let us label them. So, that it is easier for us to identify. So, I am going to label them as A, B, C, D, E, F, G right. Now, if I have to figure out which is the highest energy conformation I would say that eclipsed conformations are the highest energy, right?

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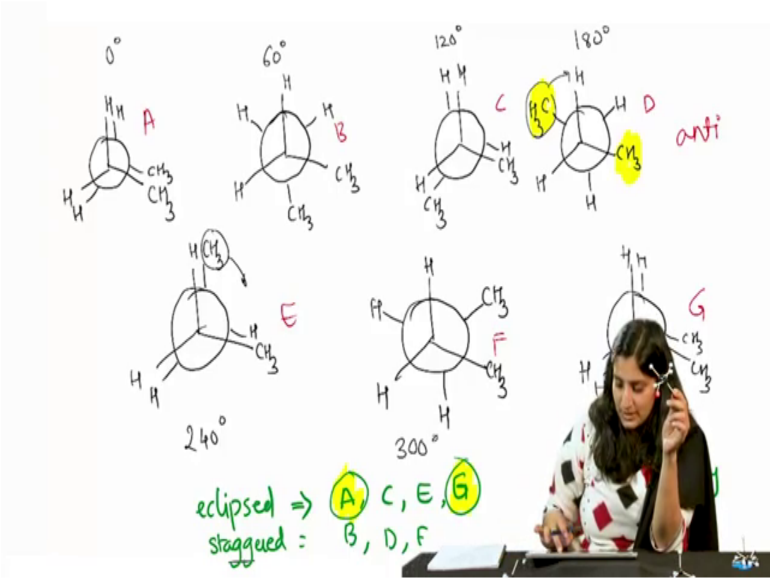

Now, there are various types of eclipsed conformations I have here. For example, in this case the eclipsed ones are A, C; A, C, E and G and the staggered ones are B, D and F, okay. Now, are all the eclipsed conformations the same? So, if I look at A, C, E and G are all of them of the same energy? The answer to this question is no, right because as you can see in A and G for example, you have 2 methyls eclipsing with each other. So, in A and G you have 2 hydrogen-hydrogen eclipsing interactions and 1 methyl-methyl eclipsing interaction whereas, in C and E you have 1 hydrogen-hydrogen eclipsing interaction, but 2 methyl-hydrogen eclipsing interactions.

So, if I really have to figure out what is the energy of each of these conformations I will have to refer to a table that talks about the torsional strains that arises because different groups eclipse with each other. If I refer to the table I see that the methyl-methyl eclipsing interaction is the highest which is 2.5 kilo calories per mole whereas, the methyl hydrogen interaction is only 1.4 kilo calories per mole. So, now, if I really think about it A and G are the highest in energy, then you have C and E which are kind of lower in energy compared to A and G. So, I will kind of show that A and G are the highest in energy, okay.

Now, between C and E as you can see C and E are kind of very similar to each other such that both of them contain similar types of strains. So, their energies will be same, but remember these are still not the same compounds. These are conformational isomers of each other wherein you can get from C to E via rotation of a single bond. So, now, let us look at the staggered conformations we have B, D and F.

Now, in B, D and F if you really have a close look one of them is clearly different from the other two. It is the conformation D in which you have these two methyls going apart from each other. So, these two methyls let us say this is D, wherein the 2 methyls are farthest apart from each other. This particular conformation which is of the lowest energy, okay because firstly, it is all staggered and the 2 methyls are farthest apart from each other is called as an anti-conformation, okay.

So, an anti-conformation is the most stable conformation because the 2 methyls are farthest apart. If you look at B and F, now, in B and F what you have is something like this, okay. So, this is for example, currently B, okay. Now, in B and F if you can see these two methyls are still in the close vicinity of each other they are not eclipsing, but they are in the close vicinity because they are staggered with each other. This particular methyl group occupies a space, okay remember we are not showing the actual methyl group, but if I had to really show it remember there would be carbon – hydrogen bonds here same way there would be carbon – hydrogen bonds here and they would clash with each other.

So, this would experience some kind of steric strain that will be rising because I am kind of trying to force this molecule to be in a conformation whereas, these two methyl groups do not want to be very close to each other. Of course, this energy will be lower than the eclipsed conformation because in eclipsed there is absolutely no space. In this case, this is called as a gauche interaction. In the case of gauche interaction, you have a little lesser strain than an eclipsed interaction, but it is still a strain and in order to refer to what kind of strain gauche interactions put with each other you can refer to this part of the table. So, as you can see a methyl-methyl gauche interaction will be close to 0.8 kilo calories per mole. So, B and F will be a little more strained than D.

So, now if I want to plot a graph of all of these;

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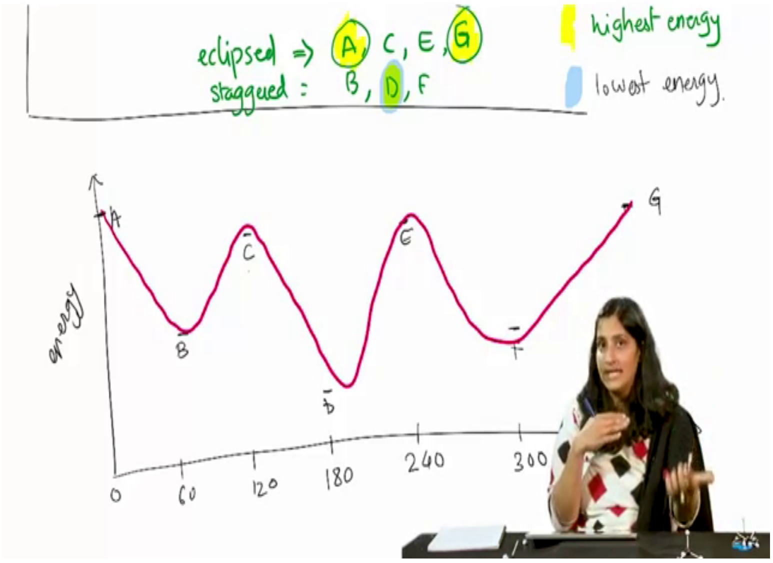

Okay, now remember we have to plot all of these A, B, C, D, E, F, G such that they fall on the energy axis. Now, A and G are the highest energy; A belongs to the dihedral angle 0 degrees and G belongs to the dihedral angle 360 degrees. So, I will place A here at the highest point and G also at the highest point. A and G are the same as each other because we complete one full rotation and get back to G. So, they will have the same energy.

Now, from A when we go to B, remember it's a staggered one and there is a gauche interaction. So, the energy of B will be a little lower, okay. From there when we go to C; C is an eclipsed one, but in the case of C the 2 methyls are not eclipsing with each other. So, the energy will be a little lower than A, but more than B, okay. So, C will be here. When we come to D, D which is the anti-conformation such that the 2 methyls are farthest apart, D is the most stable conformation.

So, D I will put at the lowest possible energy and then again C and E will be very similar to each other and B and F will be very similar to each other. So, now, if I draw the graph it would look somewhat like this, okay. So, as you can imagine the energies of these conformations are going to put a strain and that strain will vary as we go through each conformation.

Now, if we really have to calculate the amount of strain that gets put on as we move through this particular conformations, you can imagine that A which has the methyl-methyl eclipsing interaction will be highest in energy. In fact, it is close to 5 kilo calories more per mole more than D, okay. You can refer to the following graph and really look at the energies of A, B, C, D, E, F, G and really correlate it whether you get to the same numbers by looking at the corresponding table.