Introductory Organic Chemistry
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Lecture – 11
Nomenclature of Alkanes, Cycloalkanes & Bicycloalkanes

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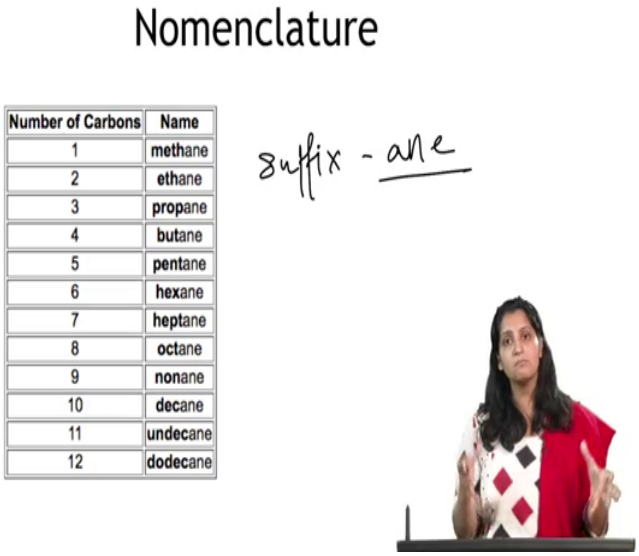

Okay, so now, we are going to look at the Nomenclature of Alkanes, Cycloalkanes and Bicyclo compounds. So, ideally every organic compound should have a name, from which the structure can be known. And also remember that it has to be a unique name, because for every compound, if there is not a unique name, then there will be ambiguity and there will be a lot of confusion. So, chemists decided to use a set of rules such that, we can come up with the unique name for a particular compound. So, for this purpose, the rules were set by International Union of Pure and Applied Chemistry or IUPAC.

I am pretty sure that you have seen the nomenclature of alkanes before and we had said that any name of an organic compound really contains a prefix and suffix. The prefix indicates the number of carbons or their arrangement in this particular molecule and a suffix indicates the functional group. So, we have kind of said that, the prefix really is your given name, but whereas, the suffix really tells you the family name or the family or the surname kind of a thing to which you belong to.

So, in the case of alkanes, we had said that the suffix is ‘ane’. So, all of the alkanes end with ‘ane’, that’s the suffix and the prefix really changes based on how many carbons are there in the compound. So, in this case we have put in a table of nomenclature as you can see, it goes from methane to dodecane and methane, ethane, propane and so on.

Really combining the prefix and the suffix together to give the name to a particular alkane. But remember, we also said that, alkanes are not just straight chain compounds, they have branched chain, they are constitutional isomers that we looked at. This now we need to know, how to name a constitutional isomers of a particular alkane or whenever there is a branched compound, how do we go about naming it such that, we get a unique name for that particular compound.

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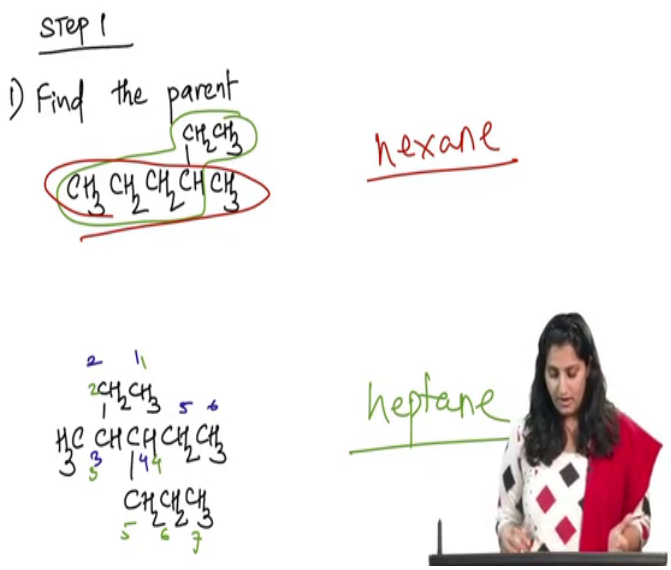

So, now let us look at, how to name a branched alkane. The first step is finding the parent, okay. Now, in this case, what we need to do is we need to find out the longest continuous chain of carbon atoms present in the molecule. Remember that it may not be a horizontal chain always and you may have to look at the molecule by turning the corners and figuring out which one is the longest continuous chain.

So, in this particular case, I have a chain that goes like this. Okay again, it has to be a continuous chain or I have a chain that goes like this, okay. If, I count the number of carbons in the green one, it has number of carbons as 6. If, I count the number of carbons that is a kind of circle with the red pen, you can see that, it only has 5. So, in this case this will be

named as a substituted hexane. Again, hex meaning 6, ‘ane’ meaning alkane. So, this will be named as some substituent of hexane.

So, now, let us figure out for the second problem. If you see, I can start numbering from the top 1, 2, 3, 4, 5, 6 right or I can start numbering from the top and go down as 1, 2, 3, 4, 5, 6, 7 okay. So, when I take that particular chain there are 7 carbons. So, what I think is in this case, the green one wins and what you have is, it is a derivative of a heptane okay, and not hexane okay. So, if I take the blue one it gives me 6, if I take green one it gives me 7, I have to go with the longest continuous chain.

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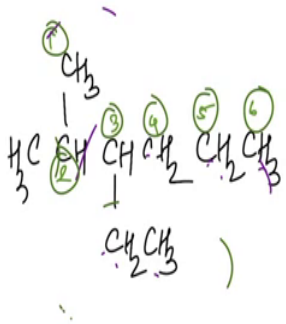

Now, let us look at some more details of this particular rule. If there are, different chains of equal length, okay. So, let’s say, I have two chains which are of equal length, how do I choose which one? So, if that is the case, then what we do is we choose the one with the largest number of branch points as the parent okay. So, for that I am going to use this particular example. Let me take this particular example here, I have 1, 2, 3, 4, 5, 6 as one of the chains or I can have 1, 2, 3, 4, 5, 6. So, what I see here are two continuous chains, both of them have 6 carbons in it, which one do I choose? If I choose the one in the purple, I have one large substituent that look like this. If I choose the one in green, I have two substituents, one is here and one of them is here.

So, if I choose the one with green one, I have two substituents and what we said is we want the one with the largest number of substituents possible. So, in this case the green one wins

and I will start numbering it such that, I use the green numbering, okay. So, I am going to get rid of the purple one. So, that is the numbering I want to follow, I want to follow 1, 2, 3, 4, 5 and 6 as the numbering for this particular alkane, okay.

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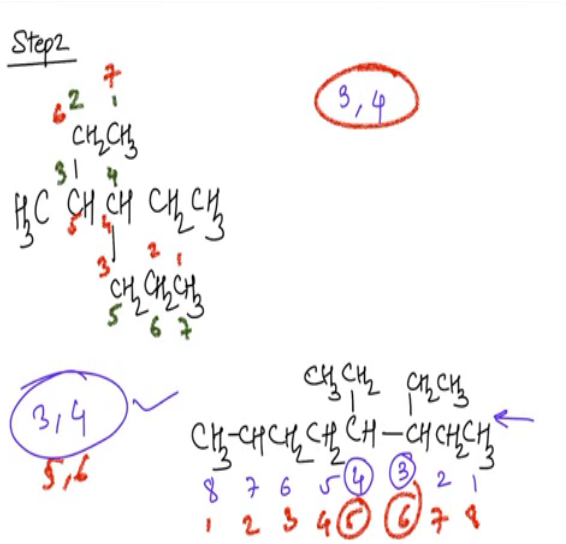

Now, let us get to our step number 2. So, step 2 talks about, numbering the atoms in the main chain. Now, what we are going to do is first figure out the parent chain and then we are going to number it. But while numbering, remember that you want to begin at the end closer to the first branch point, also remember that the substituent should have the least possible number assigned to it, okay.

So, in this case I have a heptane as my main chain right. So, what I am going to do is, let's start numbering. So, I have 1, 2, 3, 4, 5, 6, 7 okay, that's the main chain. Now, I can number it as I have shown it here or I can number it such that I start from this end 1, 2, 3, 4, 5, 6, 7, okay. Now, if I use the lettering in green, what you will see is that, it has substituents at position 3 and 4, whereas if I use the lettering in red what you can see is it has substituents at 4 and 5.

Now, remember we want it at the lowest possible number. So, the numbering in green will be better such that, I have substituents at 3 and 4 and I can discard the numbering with a substituents at 4 and 5, okay. Let us try to do this one here. Now, in this case, I have the longest chain 1, 2, 3, 4, 5, 6, 7, 8; 1, 2, 3, 4, 5, 6, 7, 8 okay; 1, 2, 3, 4, 5, 6, 7 okay. So, now, in this case, I have the longest continuous chain in this manner 1, 2, 3, 4, 5, 6, 7, 8, okay.

So, you have an octane as a chain. Now, I can go with the numbering in blue or I can start numbering it with from this end 1, 2, 3, 4, 5, 6, 7, 8. If I use the numbering in blue, what are the substituents, there is a substituent at 3 and a substituent at 4. Meaning this will give me a substituent at 3, 4. Whereas, if I use the one in red, now in the case of red there is the substituent at 5 and there is the substituent at 6. Again, you can guess that this one will be better. Okay, so, I am going to start numbering the chain from this end not from the other end.

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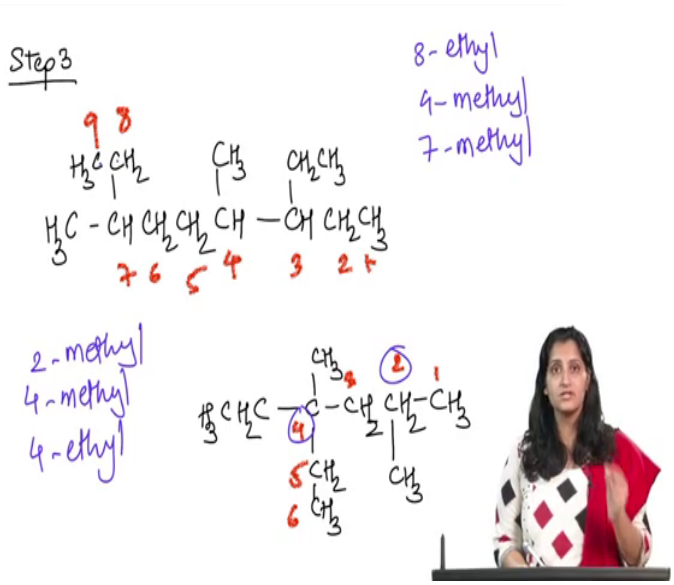

So, now let us get to step 3. Now step 3 talks about, identifying and numbering the substituents, okay. So, we are going to assign the number to each substituent and associate it to really the point of attachment. So, in this case let us, try to name this particular compound, first let us figure out the longest continuous chain, you have 1, 2, 3, 4, 5, 6, 7, 8, 9 as the number of carbons okay.

So, now let us try to solve this particular problem. In this case, you have 9 as your parent carbon. So, in fact, you can start from here, which will give you 1, 2, 3, 4, 5, 6, 7, 8 9 okay. Now, if I see on the third carbon, there is an ethyl group. Whenever there is a substituent you end it with 'yl', because it is not a complete alkane, but it is the part of the alkane right. So, in this case you have 3 ethyl, you have 4 methyl and you have a 7 methyl group okay; is it good, okay.

Now, let us try to do this one here, I have 1, 2, 3, 4, 5, 6 as the longest continuous chain. And now in this case, you have 2 methyl group, you have a 4 methyl group or a methyl group at position number 4, right. And then, there is also an ethyl group on the same carbon, which is carbon number 4, okay. So, now, we have looked at how to identify and number the substituents and also write them down. If there are two substituents on the same carbon, then we give them both the same numbers. So, like in this case on carbon number 4 we had two groups, methyl and ethyl and both of them will have the number 4 associated with them, okay.

Now, let us come to our final step, which is step 4, which really talks about how to combine all of these information together and put it together as one name. So, when we have to write down the name, remember we write it as one single word, okay. We use a 'hyphen' to separate different prefixes and we use a 'comma' to separate numbers or to separate two numbers. We start with the first letter capital; rest of the name will have all small letters. If two or more identical substituents are present, then we use one of the multipliers, such that di, tri or tetra, before them or we use di, tri, tetra prefixes accordingly.

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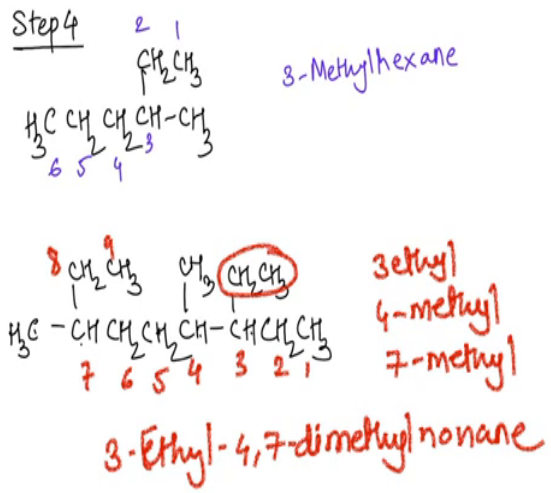

So, now let us try to write them down. Now, in this case, I can have 1, 2, 3, 4, 5, 6 as the parent carbon, that is the longest continuous chain. So, while naming it, what I am going to do is 3-Methylhexane, okay. So, the continuous name of this particular alkane is 3-Methylhexane.

Now, let us try naming this one, I can name it as 1, 2, 3, 4, 5, 6, 7, 8 and 9. So, it is a nonane derivative okay. So, I write that down as nonane. And now what you can see is, I have a substituent at position 3; which is 3-ethyl, I have a substituent at position 4; 4- methyl and then a substituent at position 7; 7-methyl okay. So, if I want to write down a continuous name of this particular thing, I go alphabetically, so, 3 will come before 4 and 4 will come before 7; 3-Ethyl-4,7-dimethylnonane.

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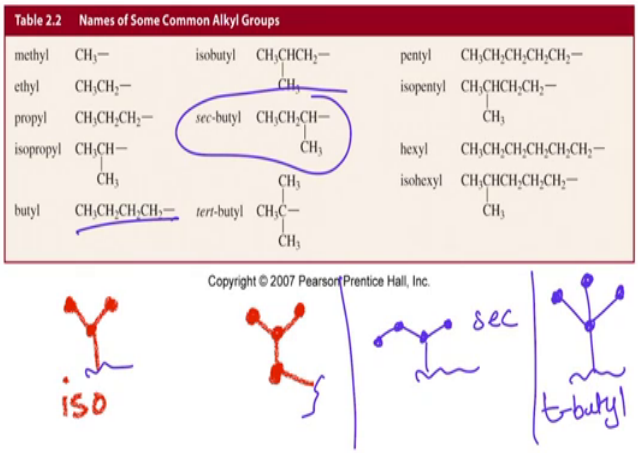

And for common names, I have a chart here. In fact, some of the common alkyl groups are in this chart, what you can see is that, the methyl, ethyl, propyl, we have already seen. But when you have a branch like this, like a Y type branch; typically, it will have a prefix as isopropyl. So, there are three carbons in this particular chain 1, 2 and 3 and here in, where it gets attached to the main, main parent carbon.

So, if I have a Y type branch coming out from, parent carbon then, that becomes an isopropyl substituent, okay. When we look at, four carbon compounds you can see that, of course, there is a butyl substituent which is all linear, but you also have isobutyl. So, how will an isobutyl look? An isobutyl should have a Y type branch, okay. And that will be 1, 2, 3 and 4 carbons, butyl because it has four carbons and it also has that Y type of branch at the end, okay. You can also have a secondary butyl attached.

So, in the case of secondary, what you see is that, for secondary, if I have four carbons like this, the main chain gets attached to the second carbon here. So, this is no longer of Y type

chain, but it has 1, 2, 3, 4 and on a second carbon you get it attached. So that, this will be a secondary butyl, okay, something like this okay. For a tertiary carbon or a tertiary butyl group, what you have is the main chain or the parent chain is attached to a tertiary carbon on the substituents. So, in this case you have 1, 2, 3 and 4 and what you have is a t-butyl group, okay.

So, it would be great to know at least the common names of 3, 4 and 5 carbon chains. So, in the case of isopropyl, isobutyl, secondary butyl, n-butyl, you also want to know tertiary butyl or when we go to pentyl, now what you have is a pentyl, isopentyl, secondary pentyl and a neopentyl group that can be used. So, all of them are in this table. And you can see them and try to use them; sometimes it is ok, to even use a common name as the substituent group, okay. So, we will go over with more examples in our tutorial.

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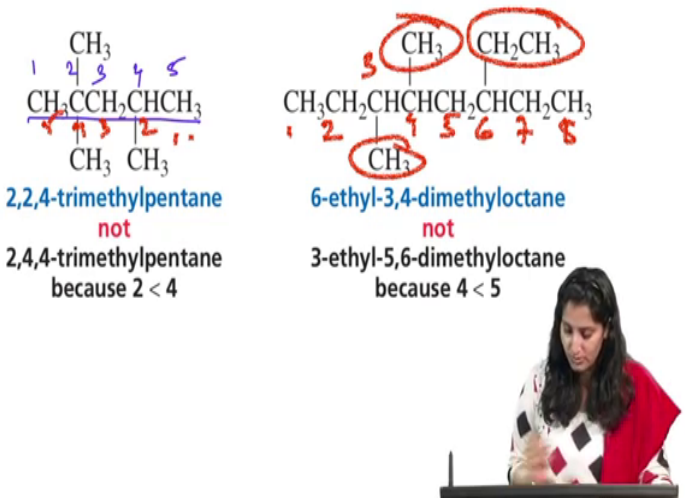

So, I have some of the solved examples here. And what you can see is that, it just goes through, why one particular name is better or is correct than the other one? So, in this case, this is the trimethylpentane. So, this is going to be the parent chain. Now, I can start numbering it from here, so from 1, 2, 3, 4, 5 right, now that will give me a substituent on, two substituents on 2 and one substituent on 4. If I start going it or if I start numbering it, the other way round as 1, 2, 3, 4, 5 that is wrong, because that gives me 2, 4, 4 which is wrong, because 4 is more than 2. So, in this case numbering in blue is better.

Let us look at one more example here. So, this is an octane derivative, so I can start numbering from here 1, 2, 3, 4, 5, 6, 7, 8; that's an octane. Now, there is a methyl here and a methyl here right and that gives me 3, 4-dimethyl and it also gives me 6-ethyl substituent. So, the numbering will be 6-ethyl-3,4-dimethyl. If I start the other way round, it will be 3-ethyl and 5,6-dimethyl. Again, if I look at the lowest possible number, then this one is better, so it will be 6-Ethyl-3,4-dimethyl compound.

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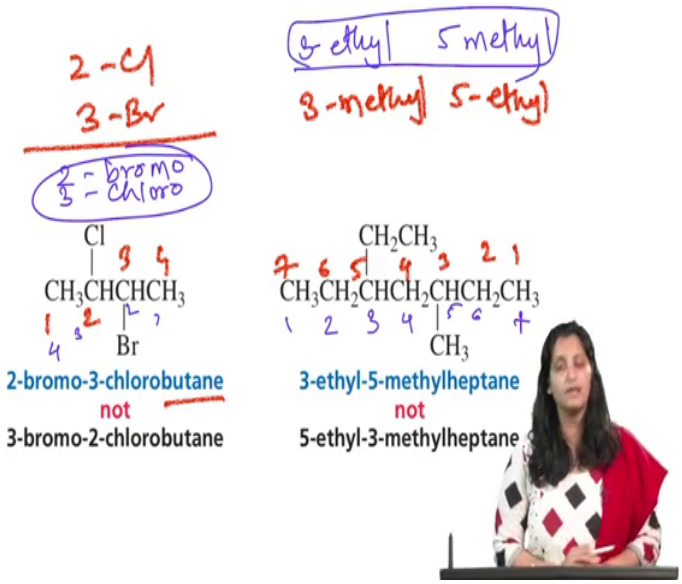

Let us look at, alkyl halides. In the case, halogen is attached to the carbon, the naming is exactly the same, there is no priority given to the halogen. So, what you can do is, you can follow the same rules, for naming alkyl halides as well. In this case, if I start numbering 1, 2, 3, 4 it's a butane derivative so, that is correct.

Now, I can start numbering such that, chlorine gets a position 2 and bromine gets proposition 3, okay. So, it will be 2-chloro 3-bromo that is one option or if I start going other way round, which is 1, 2, 3, 4 then, it will be 2-bromo 3-chloro, okay. In this case, this one is definitely better, the blue one, because bromine is alphabetically before chlorine. So, 'b' comes before 'c' and what you have is the lowest position, given to bromine because it is alphabetically better than chlorine, okay.

So, now let us do one more example here; I have a heptane derivative, what I have here is 3-ethyl 5-methyl that is one of the possibility or it could go like 5-ethyl 3-methyl, okay. So, it could be 1, 2, 3, 4, 5, 6, 7 or I could go the other way round and it will be 1, 2, 3, 4, 5, 6, 7. If

I, number it in blue, I get a 3-ethyl 5-methyl and if I number it in red then I get a 3-methyl 5-ethyl.

Now, you might ask question, that both of these numbers are same. So then, which one to prefer? Always remember that, we have to go alphabetically. So, since ‘e’ comes before ’m’, the substituent with the ‘e’ or ethyl should have the lower possible number associated with it. So, what I have is 3-ethyl-5-methyl.

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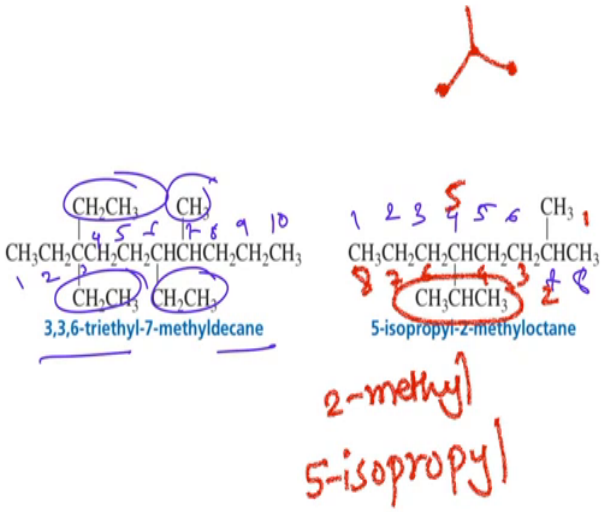

Again, you can see here I have solved some of these examples, you have 3,3,6- Triethyl. So, you have 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 so, that’s a decane. You have one two three ethyl groups, so, this one becomes 3,3,6 because they are at positions 3, 3 and 6. So, you have 3,3,6-Triethyl and then you have a 7-methyl. Okay, so that is the name. In this case now, here is one naming with the common name system.

So, what you have here, is it’s an octane 1, 2, 3, 4, 5, 6, 7, 8 okay or I can go the other way round 1, 2, 3, 4, 5, 6, 7, 8 okay, which gives me the lowest possible number to a substituent which is 2-methyl okay. So, let’s write that down, so this is 2-methyl. Now, on position 5, if you see, there is this isopropyl group, because it is attached like in the form of Y right. So, this is attached like that. So, this will be 5-isoPropyl-2-methyloctane okay.

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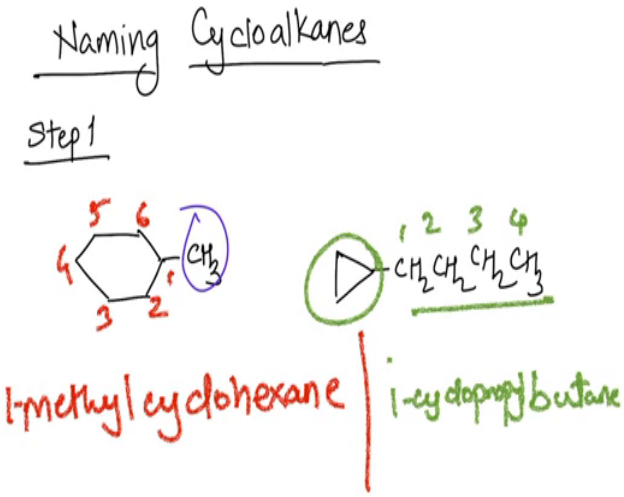

Now, let us learn how to name the cycloalkanes. Now, the rules are very similar for cycloalkanes and that of alkanes and you can pretty much use all the rules of alkanes in order to name the cycloalkane. But there is just one addition to the rule of cycloalkanes. Now, remember cycloalkanes will be such that you have cyclopropane, butane, pentane and so on, but you can also have substituents or alkyl substituents to these cycloalkanes.

So, then in which case we want to do decide, whether this particular compound can be named as a cycloalkane with an alkyl substituent or whether it can be named as an alkane with the cycloalkyl substituent. So, in order to decide that, what we do is, we count the number of carbons that are there in the ring separately and we count the number of largest substituents that are, that the particular compound has, and we count the number of carbons in that substituent.

Now, if the number of carbons in the ring is greater than or equal to the carbons in the substituent, then it will be named as a alkyl substituted cycloalkanes. So, cycloalkane will become the parent chain, whichever one is higher in number that becomes the parent chain. Whereas in the case, if the number of carbons is higher in the substituent then what you can see is that, the compound will be named as an alkane, right and it has a cycloalkane substituent, okay.

So, let us try to look at this rule with help of this example. Now, what I have is 1, 2, 3, 4, 5, 6 right, I have 6 carbons in the chain, a cycloalkane chain, where as I have only one carbon in the substituents chain. So, this one definitely will be such that you have, this one will be

named as Methylcyclohexane or you can even add that 1, 1-Methylcyclohexane; you may not see it being added all the time, but sometimes, it is good to write it in a very correct form, which is 1-Methylcycloalkane.

Now in this case, the other case, when I want to write it down, as you can see, you have 1, 2, 3, 4 right. There are 4 carbons in the substituent, but whereas there are only 3 carbons in the cycloalkanes. So, in this case, this will be named as 1-Cyclopropylbutane okay. So, in this case, our parent becomes the butane and it will be 1-Cyclopropylbutane.

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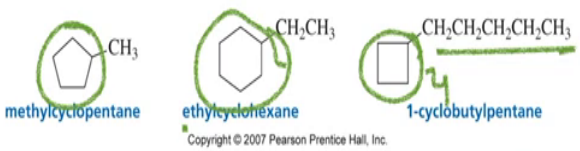

So, I have some more examples here, you have methylcyclopentane. Again, because cyclopentane has more number of carbons, this will be ethylcyclohexane, okay. Now, in this case, there are 4 carbons in the cycloalkane part, but there are 5 carbons in the pentane part or the substituent part. So, this will be 1-Cyclobutylpentane, okay.

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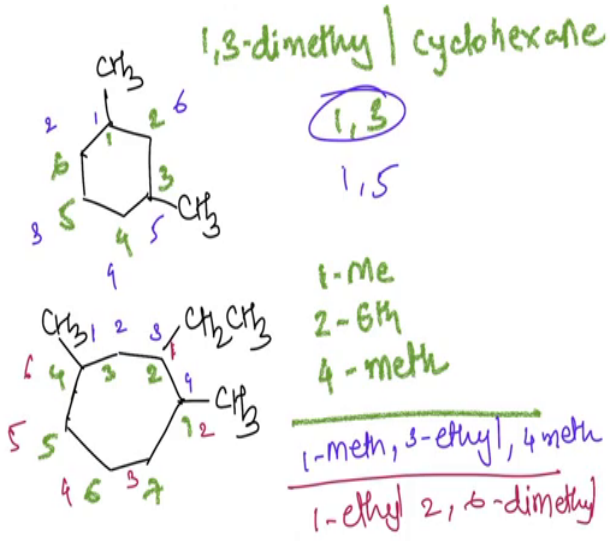

Now, let us look at the second rule of naming cycloalkanes. In this case, what we do is, we number the substituent such that, the substituent gets the lowest possible number, which is the same rule as in the case of alkanes. But in the case of cycloalkanes, you also want to remember is that, if you start numbering such that you start going in a clock wise direction, you follow it throughout. Or if you start numbering such that, you are going in anti-clock wise direction, you still follow it throughout. So, you cannot change directions in between, if you start going clock wise, stay clock wise. Now, whether to go clockwise or anti-clockwise is really dependent on where are the substituents. So, let's look at this particular case.

Now, if I want to name this particular cyclohexane, first of all the parent will be cyclohexane. And I have two methyl groups. Now, I can start naming them, such that I start from 1, 2, 3 okay, 4, 5, 6 that is one way of naming or I can start such that, I go 1, 2, 3, 4, 5, 6. If I use the green way of naming, I can have substituents at 1,3. If I use blue way of naming, I can have substituents at 1,5 right, so; obviously, we do not want 1,5 because I can have the same name with the lower possible number associated with it. So, the 1,3 will be better and a name of this particular cyclohexane will be 1,3-Dimethyl cyclohexane, okay.

Now, let us go to the next example. In this case, I can start labeling it such that, I can go 1, 2, 3, 4, 5, 6, 7 okay, that gives me 1-methyl, okay, I am not writing the complete name, 1-methyl, 2-ethyl and 4-methyl okay. Let us try to look at another possible numbering, I can start from here and I can go 1, 2, 3, 4. So, that will give me 1-methyl, will give me 3-ethyl and 4-methyl, right. I can even number it one more way, so let us, try looking at that, okay.

So, I can start numbering it from ethyl and I can go 1, 2, 3, 4, 5, 6. So, that will give me 1-Ethyl-2,6-dimethyl.

So, if you look at all these numbers so, what we can see is 1, 2 and 4 is only possible, only when we number it such that, we have done it in the green way. The other two give me a 1, 2, 3 and 4 which is higher than 1, 2 and 4 and another one gives me 1, 2 and 6 which is also higher than 1, 2 and 4. Remember, I am not adding them up or anything, I just go 1 1, 2 2, but when I see between 4 and 6 then 4 wins over 6.

Many a times, I see students making a mistake, where they are trying to add these numbers up and they are trying to look at the sum that is not the right way. Always remember that you want to go number by number 1, 2 and 4 versus 1, 2 and 6; 1 and 2 tie with each other. So, now, I debate between 4 and 6 that is the right way of figuring out, which one is the better way of numbering.

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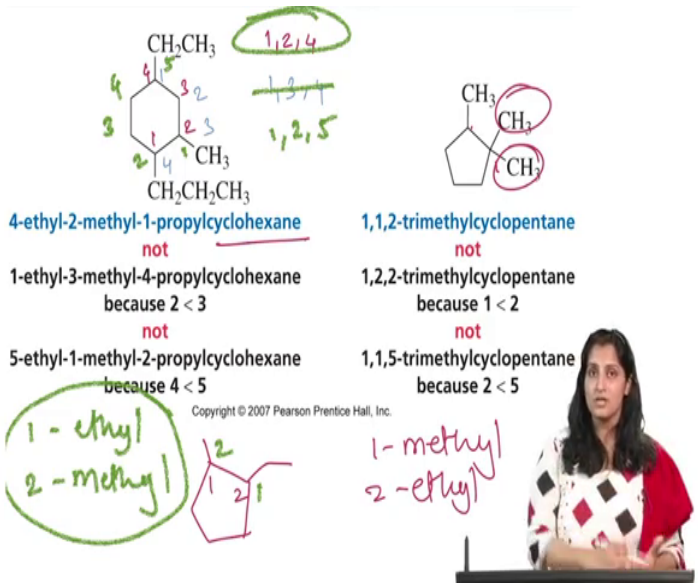

So, now what I have here is the cyclohexane. So, that is okay, then if I start numbering it I can start numbering it such that, I go 1, 2, 3, 4 that is one way, which gives me the very first option 1 propyl, 2 methyl, 4 ethyl okay. So, the numbering is 1, 2, 4. In the case of, if I start from this way, if I start from here, I can go 1, 2, 3, 4. So, that gives me 1,3,4, the blue one or if I choose the green one, I can start by numbering here 1, 2, 3, 4, 5. So, this will be 1, 2, 5 right.

If I want to really now choose between them, this one clearly loses out, because it does not have the number 2 and other two have it, so the lower one wins. Now, between 1,2,4 and 1,2,5, you want to choose one with 1,2,4 okay. So, I will choose the numbering which is the red one 1, 2 and 4. In this case for the second one if you have 1,1,2 such that, you have more substituents having the lowest possible number 1. So, it will be 1,1,2-Trimethylcyclopentane, okay. Again, in this case, also remember that you want to go alphabetically. Meaning if there is a chance such that, you have two or more different alkyl groups could potentially receive the same number. So, in this case I am going to write it like this.

Now, for this particular cycloalkane, it is a cyclopentane that is okay, but I can number it such that I go 1 and 2 such that, 1 gets the methyl group and 2 gets the ethyl group okay. Or you can also go as 1 and 2 such that, 1 gets the ethyl group and 2 gets the methyl group. Then I will choose the one in green, because that will give me the alphabetically first substituent, that is ethyl have a lower number than methyl, okay. So, when there is a clash such that, this numbering system also gives me 1 and 2, the other one also gives me 1 and 2, I go alphabetically and give priority and having the lowest possible number assigned to a substituent that goes alphabetically first.

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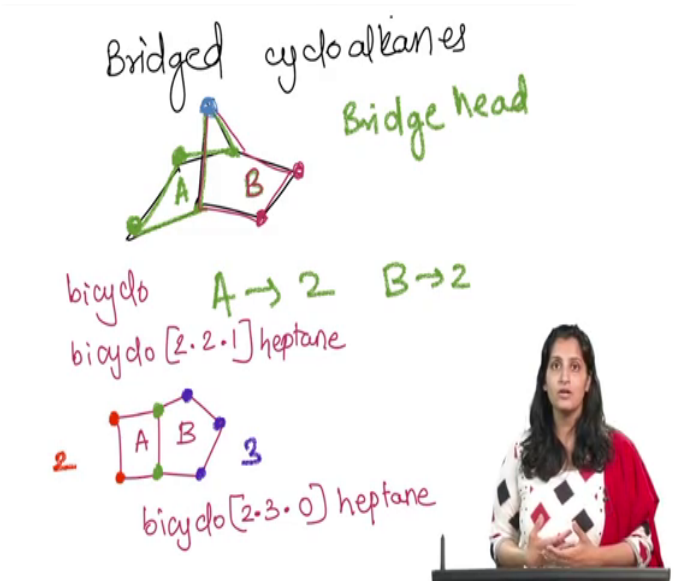

So, now what we are going to look at is, we are going to look at bridged cycloalkanes or these are also called as bicyclo compounds. So, in this particular example as you can see, you

have a compound that has a bridge in between the two carbons right. So, these two carbons are also called as bridged head carbons. Okay, so, these are the Bridge head carbons.

Now, when we want to name bicyclo compounds, what we do is, we first identify their rings. So, in this case I have two rings A and B okay; I will use a different pen. So, ring A goes kind of like this and ring B goes kind of like this, right. So that, those are the two rings okay; we also the prefix 'bicyclo'.

Now, in order to name this bicyclo compounds what I am going to do is, I am going to count the number of carbons in each ring and we are going to count them, such that ring A first then ring B and we exclude, the carbons that are at the bridge head. So, if I look at the carbons in ring A; A has two carbons, B also has two carbons. So, A has 1 and 2, B has 1 and 2 these are the two carbons each. And if you count the number of carbons in the on the bridge, there is 1 carbon which is kind of shared between these two rings.

So, now when I have to write down the name of this particular compound, I start writing bicyclo into bracket 2 dot 2 dot 1, okay. So, that is about each ring individually, but now we have to also state, how many carbons are total present in this particular compound. So, if I count the total number of carbons that comes out to be 1, 2, 3, 4, 5, 6, 7. So, this is the heptane derivative okay, this is Bicyclo [2.2.1] heptane.

Now, let us try to solve one more compound or let us try to look at one more example, okay. So, I am going to try and solve this particular compound; there are two rings of course, A and B, these are my bridge head carbons. I am not going to count them, while counting the number of carbons in each ring. As you can see, the bridge has 0 carbons. Meaning it is a direct bond between the two bridge head carbons.

So, now, what I am going to do is, I am going to count the number of carbons in the ring A. So, that is the 2 carbons, I am also going to count the number of carbons in ring B, that is 3 carbons right. So, this will be called as bicyclo 2 dot 3 dot 0, because there are 0 bridged head carbons heptane, because if you count the total number of carbons you have 7 carbons again 1, 2, 3, 4, 5, 6, 7 carbons. So that is how we name the bicyclo compounds.

So, we looked at how to name alkanes, cycloalkanes and bicyclo compounds. So, again the more you practice the better you will be at naming these particular alkanes or cycloalkanes. The rules are pretty much the same throughout any functional groups. So, when I have to

look at a different functional group like alkenes, only some of these rules change or mainly only one or two of the rules change, rest all the rules pretty much remain the same.

So, it's good to first understand, how to name alkanes and cycloalkanes and bicyclo compounds. And then in the next chapter, when we go over alkenes, we will go over the alkene nomenclature, but not in so much detail because, the rules are pretty much the same for alkanes and alkenes, okay. So, in the tutorial, do solve the more problems and also go through the solution such that, you can verify if you have a mastered the art of naming alkanes.

Thank you.