Symmetry, Stereochemistry and Applications
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Module No # 01
Lecture No # 03
Nomenclature of Cyclic Molecules and Other Functional Groups

Welcome back to the course on symmetry and stereochemistry and applications. So we were trying to understand the different rules of IUPAC nomenclature for various organic compounds. So in the previous 2 lectures we have learnt about how to write the names of organic molecules for simple hydrocarbons, substituted hydrocarbons. And then we also learnt about the naming of alkenes.

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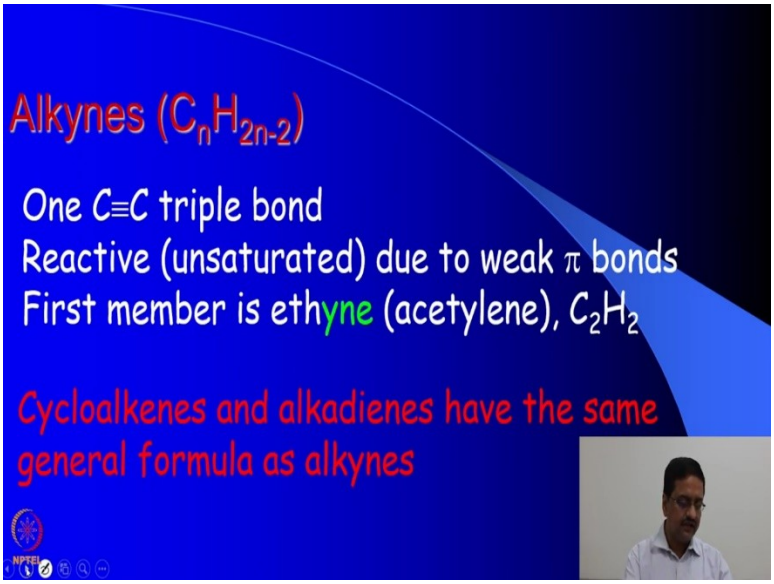

So in that direction we would continue to understand the names of alkynes. As you know the alkynes are the compounds which contain a C-C triple bond and these are as usual reactive in nature due to weak Pi bonds. The first member of this series is the ethyne or acetylene which is identified as C2H2. But you can understand that there may be a large number of different compound which can have C-C triple bond.

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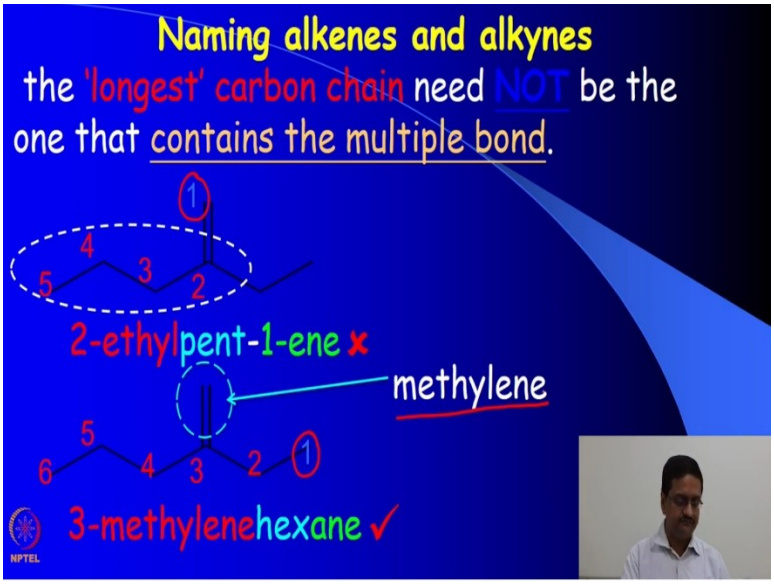

And you may have notice that cycloalkenes and alkadienes have the same general formula as alkynes. So we will continue understanding the names of alkynes and alkadienes in these upcoming slides. So we will first see what happens when you have different types of alkenes and alkynes connected together. So the first point that again and again we should remember that we need to find about the longest carbon chain.

And that longest carbon chain need not be the one which has the multiple bond. So for example in this particular case you have a molecule written here in the upper portion where you can number the atoms starting at the point where the double bond starts. And then number it like 1, 2, 3, 4 and 5 as is shown in the upper structure. And you can try to write a name like that 2-ethylpent-1-ene. But you see in these particular case the longest chain is neglected.

The longest chain is formed by numbering it from this particular end where you have 1, 2, 3, 4, 5 and 6 so it become hexane. And this substitution that is here is a methylene substitution. So when you try to write the name of this compound we do not take the longest chain containing this C=C double bond rather we take a longest chain which is not containing the double bond. And the double bond is outside the chain. So we write this as 3-methylenehexane.

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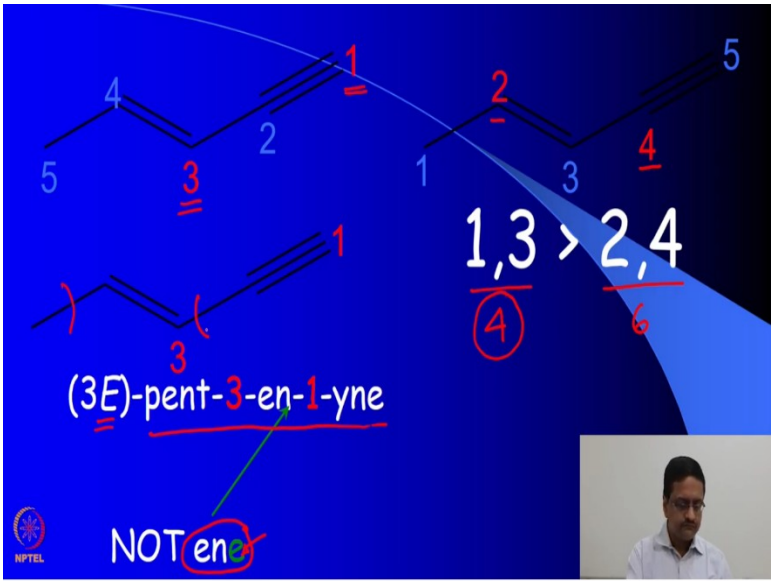

Now you see in these examples we have a situation where we can identify a double bond and the triple bond in the molecule. And depending on from which side we tried to number those double bonds and triple bond gets different numbering. So when you try to number it from the right hand side giving priority to the triple bond the number gets 1, 2, 3, 4 and 5. So number for the triple bond and double bond is 1 and 3.

Whereas if you try to number it from the other end then the position of double and triple bonds get numbering 2 and 4. And here we need to remember that the sum of these two numbers should be the lowest for a correct numbering. So in case of the left one we have 1 and 3 which is, the sum is 4 and in the right hand side it is 2 and 4, the sum is 6. So this sum gets priority over the other one. As a result we write the name of this particular compound as pent-3-en-1-yne.

You must notice 2 things, number 1 when I am writing en designating the double bond. Instead of ene we are writing only en we have dropped that particular e. And we also have identified the double bond as e which is entgegen that is in opposition to because about this double bond these 2 groups are on the other side, opposite sides of each other making it so called trans and in this particular case we write it as E.

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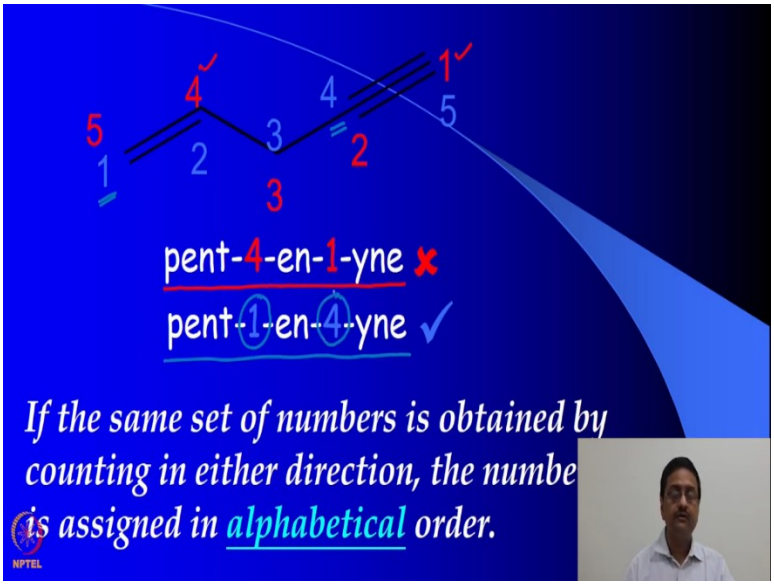

Now we have a different situation here. What we have is a molecule where at 2 terminus we have a double bond and a triple bond. So there are 2 different ways of numbering it. We can make it as 1, 2, 3, 4 and 5 from the right hand side or 1, 2, 3, 4 and 5 from the left hand side. So when we write it in the way that the 1 identifies the triple bond and 4 identifies the double bond the name should have been pent-4-en-1-yne.

Whereas if we write it in a different way with double bond getting priority 1 and triple bond getting position 4 we can write this name with giving this double bond priority as 1 and triple bond priority as 4 and write the name as pent-1-en-4-yne which is the correct nomenclature that we need to know. So here the rule is, if the same set of numbers is obtained by counting in either the direction the number assigned in the alphabetical order. So en comes before yne. So en gets number 1 and yne gets number 4 and that is why we write pent-1-en-4-yne as the name of this molecule.

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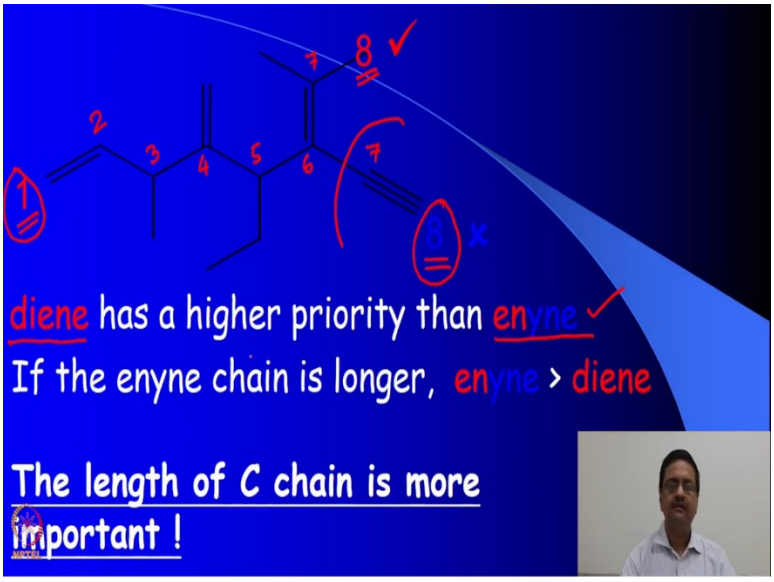

Now we have a slightly difficult molecule. You can see here in this particular molecule we have 3 double bond and 1 triple bond. There are many different ways one can start numbering it and from the previous slide, we have understood that if we have en and yne we should give priority of en above yne. So we should start numbering from the end where the double bond is numbered 1 and triple bond is numbered the lowest.

Now we can come from this end and write the number 1, 2, 3, 4, 5, 6. Now we need to see whether we should go towards that or towards this. So here you have 2 possibilities going up or coming down towards the triple bond. So again now we again refer to a new rule where we learn that diene has a higher priority over enyne. So if we write the numbering from 1 to 8 on the en side then it is named as diene and that yne is a substitution.

If we write it from this 1 to that 8 then it becomes enyne and that gets a side chain. And the rule says diene has a higher priority over enyne. So we should number it in the way as shown as above.

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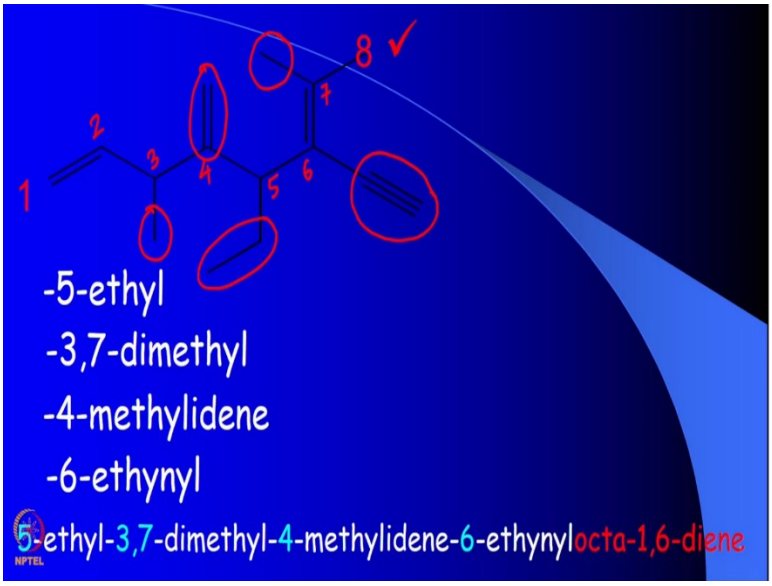

So now let us try to understand what the name of this compound should be. The previous slide we have clarified how the numbering of the longest chain should be done. So here what I have shown is the numbering of the carbon atom starting from the left corner to the right corner with 1, 2, 3, 4, 5, 6, 7 and 8. So what we have here is at 5 position we have the ethyl group at 3 and 7 position we have 2 methyl group as you can see. At 4, position we have a methylidene group.

At 6, position we have this ethynyl substitution. So what we should name this molecule as is written here at the bottom of the slide 5-ethyl-3,7-dimethyl-4-methylidene-6-ethynylocta-1,6-diene. So this is how we should try to understand and write the name of a hydrocarbon or a complicated molecule where you may have two or more double bonds and triple bonds present in the molecule.

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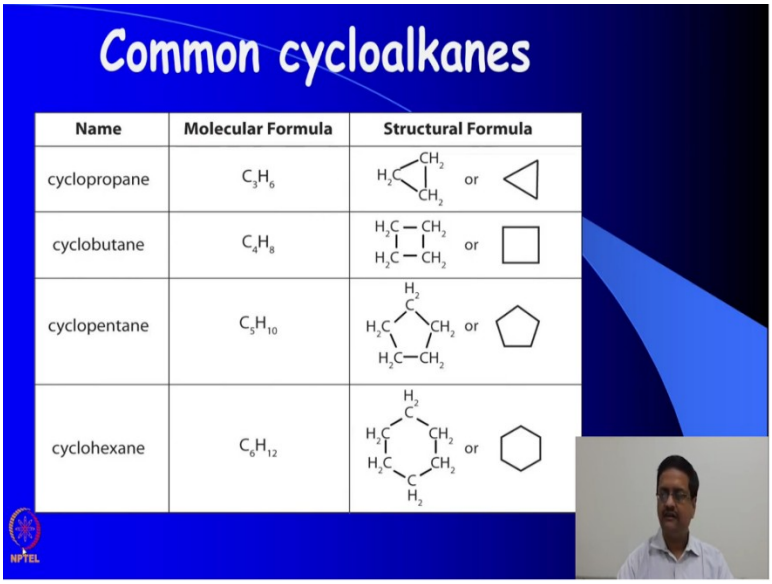

So when you learn about cyclic alkanes there are few very commonly encountered cyclic alkanes as I have shown here cyclopropane, cyclobutane, cyclopentane, cyclohexane etc., These are very common cyclic compounds that we encountered in our organic chemistry courses.

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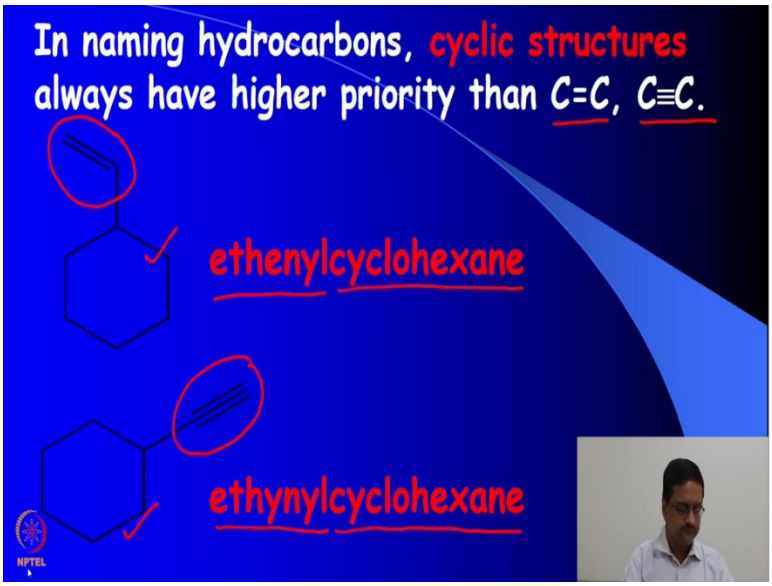

So when we try to name those cyclic structures, so the cyclic structures always have higher priority over C double C or C triple bond C. So this should be named as ethenyl is the substitution and cyclohexane is the parent that we have inside. Similarly, ethynyl is the substitution and cyclohexane is the parent that we have here.

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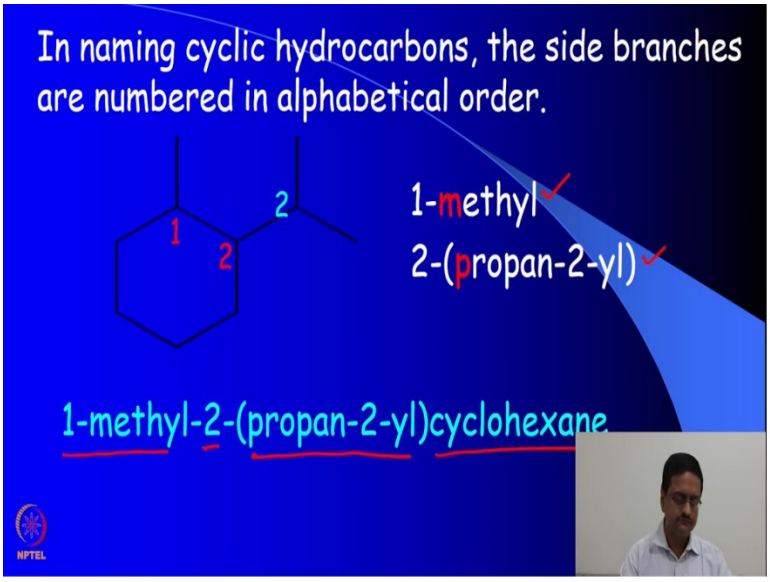

So when we try to name the cyclic hydrocarbons the side branches are numbered in alphabetical order. So now we have 2 substitutions in this particular molecule and methyl substitution and a propan-2-yl substitution. So while numbering it we should have give methyl first priority because m comes before p. So we write is as 1 methyl at 2 position we have propan-2-yl because this is a three membered ring connected in the middle proportion. So we write it as 1-methyl-2-(propan-2-yl)cyclohexane.

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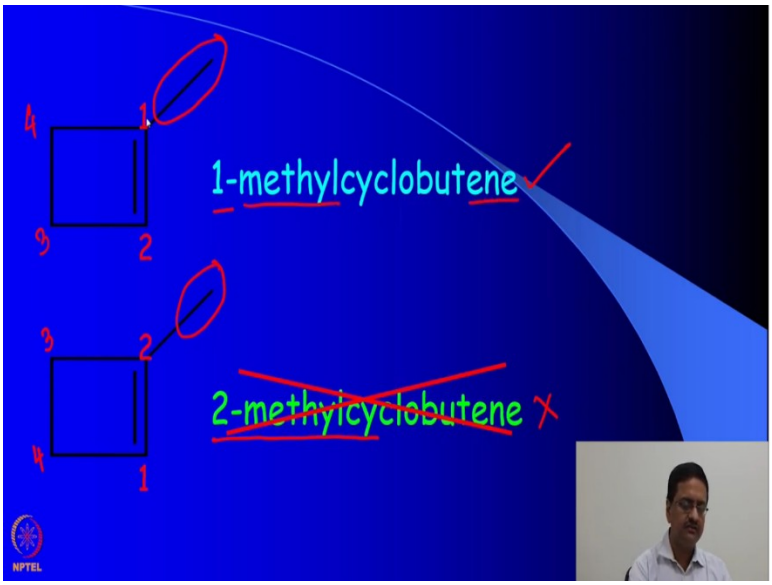

Now we see here there are 2 possibilities of writing this name. We can have a cyclobutene and we name it as 1-methylcyclobutene because the methyl group is attached to carbon 1 when I am numbering it like that 1, 2, 3 and 4. But if somebody numbers it in the opposite direction 1, 2, 3

and 4 the name should be 2-methylcyclobutene because now the methyl group is here. What do you think the name should be? The correct name of this molecule should be this one not that one because the substitution is methyl gets the lowest number and cyclobutene ene is also is at position number 1.

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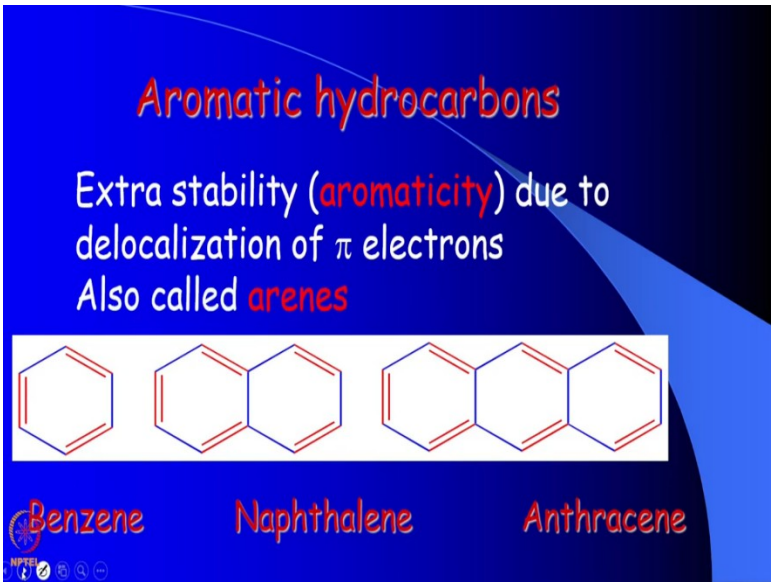

As you all know that the other class of cyclic compounds are aromatic hydrocarbons and we have molecules like benzene, naphthalene, anthracene etc., So these molecules also we need to identify with appropriate names, Because of aromaticity these molecules are more stable than some of the hydrocarbons. These are called arenes as well.

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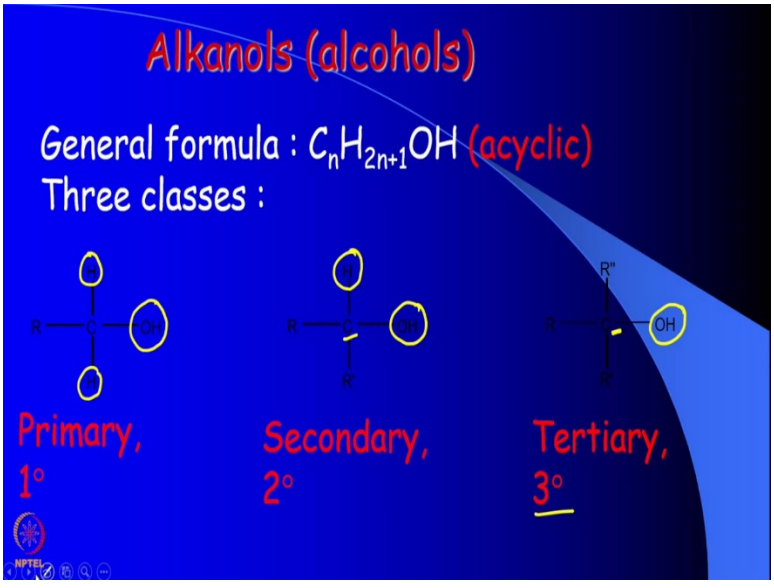

So when a group which is C6H5 is attached to any compound is called a phenyl group. Similarly a naphthalene with 1 hydrogen less is called a naphthyl group. And these are basically called the aryl groups. Then the next class of compounds that we encountered very frequently is the group of alcohols. And as you may know the alcohols can be identified as primary, secondary and tertiary depending on the connectivity of OH with the carbons.

So if the OH is connected to a carbon which has 2 hydrogens is called a primary alcohol. If the OH is connect to a carbon which is in turn only connected to 1 hydrogen is called the secondary alcohol. And if you have the alcohol the OH group connected to the carbon where there is no hydrogen atom is called a tertiary alcohol or a three degree alcohol. So it has a general formula CnH2n+1OH. So three classes of alcohols that we can think of primary, secondary and tertiary.

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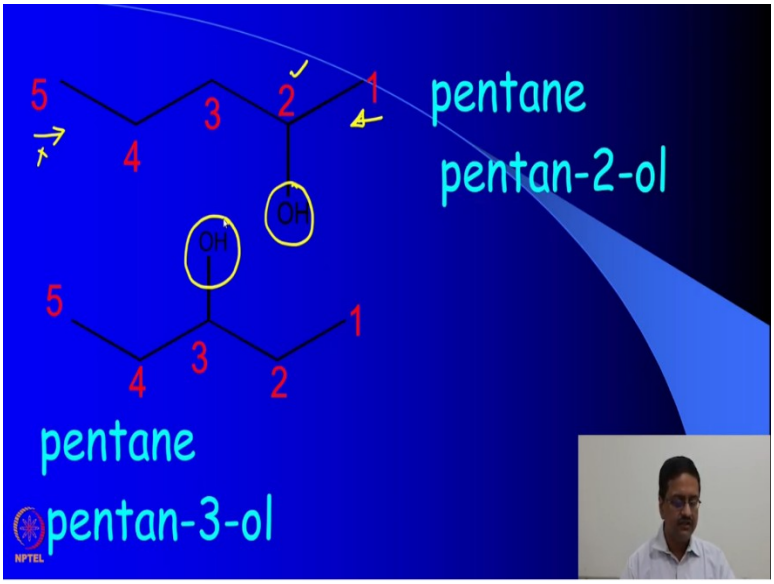

So when we try to now name these molecules, we first try to identify the long chain as usual and try to identify the position of OH group getting the lowest number. So that is why we did not start numbering from the left side rather we started numbering from right hand side and made it as pentan-2-ol. In the second case when we have the OH group in the middle it is imperative that one from either side it gets number 3. So we do not need to worry about numbering from which side or whatever so we write is as pentan-3-ol.

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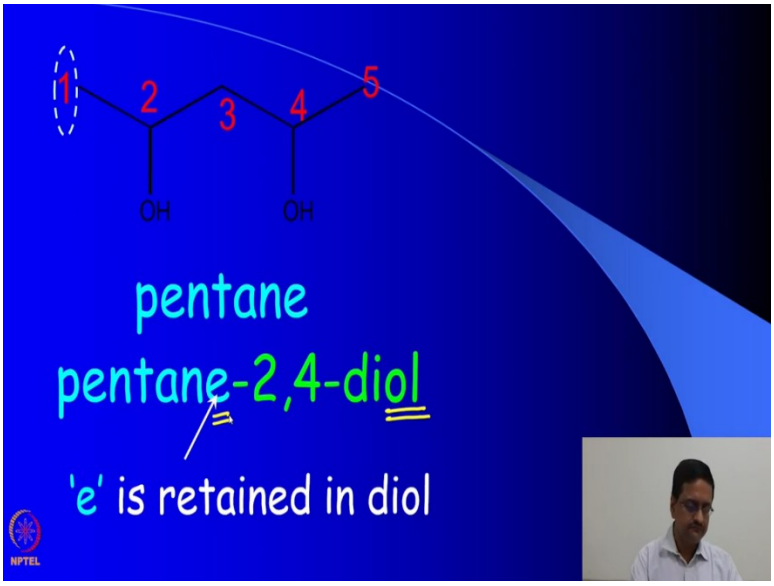

There can be a molecule where you may have 2 OH groups. So we should number the carbon chain in such a way that both the groups get the lowest priority. In this particular case from either side these numbers will be 2 and 4. So therefore the name of this molecule will be pentane-2,4-diol. So this is the family name of alcohol that gets associated is the phrase -ol identifying the presence of alcohol. Now you see that in this case e is retained in case of diol where in case of enyene that e was dropped.

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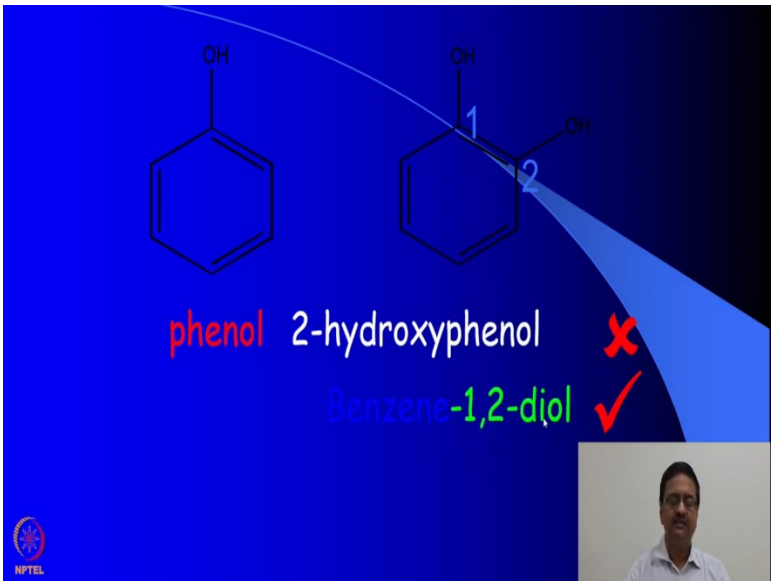

The other class of compounds containing OH group are the phenols. These are the derived from aromatic hydrocarbons and contain one or more OH groups attached directly to the aryl groups. So we write it as Ar-OH and common example of that molecule is phenol. So here you have 2

molecules which are having this OH groups one is phenol and the other one is 1,2-dihydroxy benzene not 2-hydroxyphenol. Why is that?

Because when you try to write the name you cannot give one as a priority over the other if the functional groups are same. So we write it as benzene-1,2-diol or 1,2-dihydroxybenzene and not 2-hydroxyphenol.

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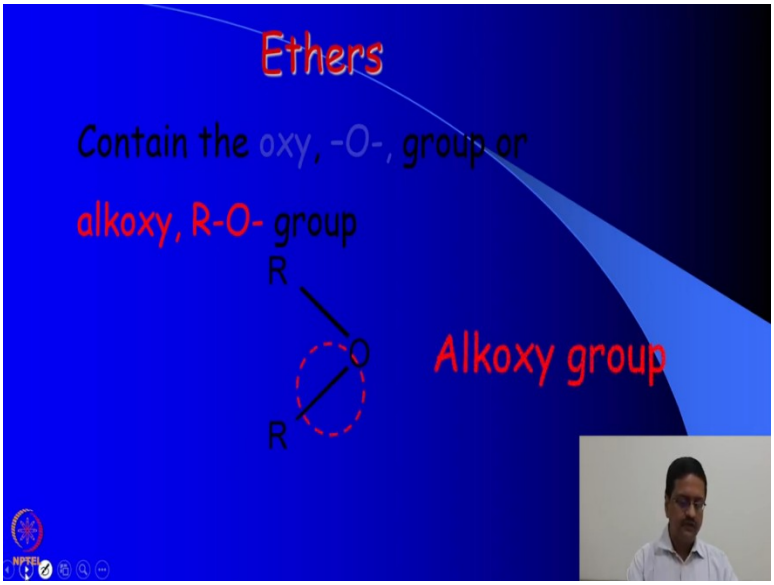

The next class of compounds is ethers where it can have 2 alkyl or aryl groups connected by 1 oxygen and these are called the alkoxy groups where you have a bond of R and oxygen.

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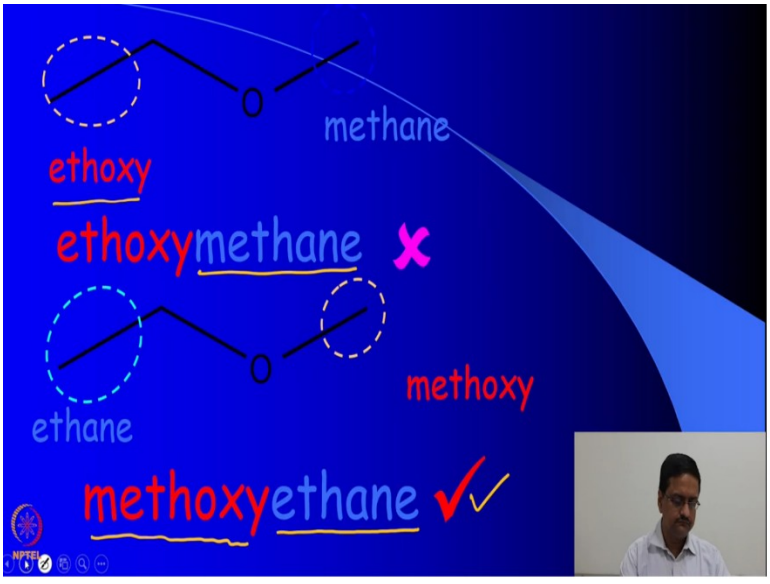

So here in this case you can see 1 molecule and we can write the name in 2 different ways. One way where we identify one group as ethoxy because you have ethyl group connected to oxygen and here it is a methyl group. So we can write it as ethoxy methane or we can write it as methoxy ethane. By now you should be able to identify which is the correct name. The correct name is the second one because here we have considered the long chain as the parent molecule and methoxy as a substitution.

So this becomes methoxy ethane instead of ethoxy methane because in that case methane is the parent which has less number of carbon atoms compared to ethane.

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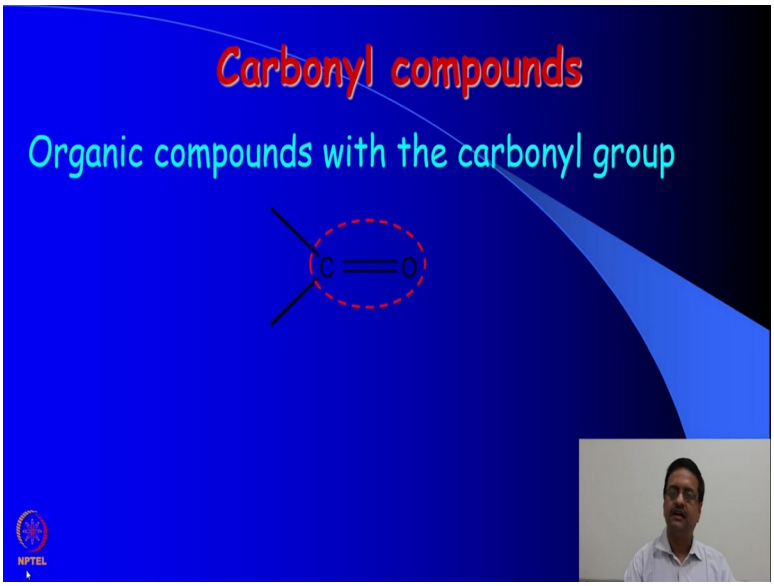

The next class of compounds is carbonyl compounds where you have C double bond O

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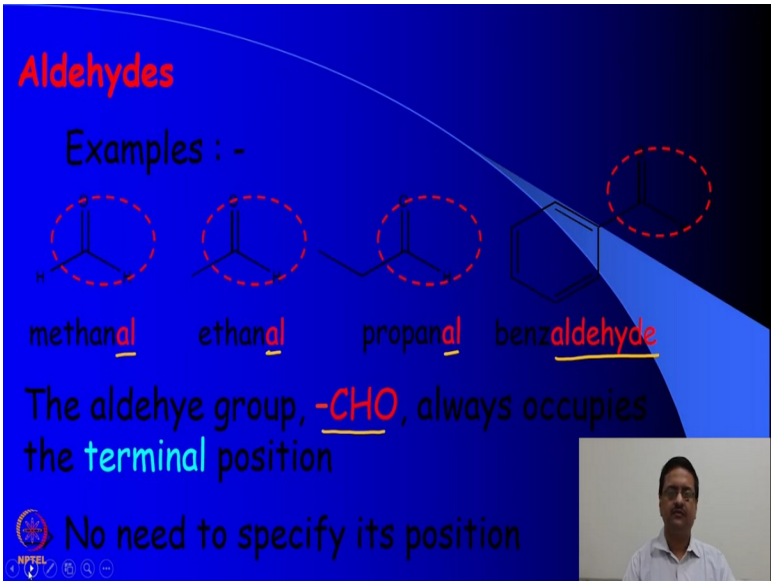

And the carbon is connected to 2 alkyl groups. So those compounds have 2 different types, can be ketones and aldehydes. So when you have 1 aldehyde you have the family written as al and in case of benzaldehyde it is written as aldehyde. So, methanal, ethanal, propanal etc., are the common names of those aldehydes that we generally encounter. The aldehyde group that is the CHO group always occupies the terminal position of a molecule.

So no need to specify the position of this aldehyde group in a molecule. The carbon atom forming the aldehyde group is always given the priority number one and we do not need to mention that in the name of that particular molecule. So we do not write as propan-1-al rather we write it as propanal.

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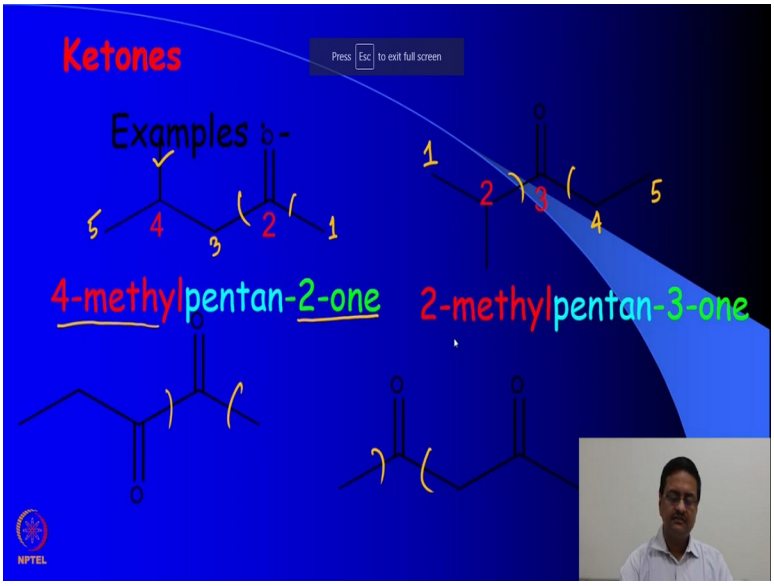

The ketones are the next type of molecules next group of molecules where the C double bonded O is associated with a carbon which has 2 carbon atoms connected to it. Everywhere if you see that you have 2 carbon atoms connected to that carbonyl group. So you can have the names following the IUPAC nomenclature, this compound the top one has 5 carbons writing the name from the right hand side 1, 2, 3, 4 and 5.

At 2 positions you have ketone so we write it as one and 4 methyl is the substitution at position number 4. So it is 4-methylpentan-2-one. The next compound that we have here is 2-methylpentan-3-one because the carbon atom at number 3 contains the ketone carbonyl group or the ketone moeity. So it is 2-methylpentan-2-one.

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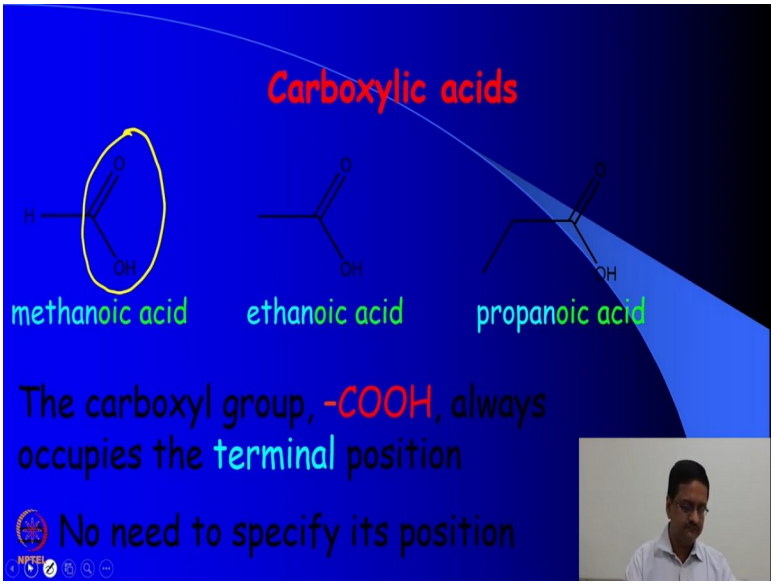

So I leave the other 2 ketone for you to identify the name of those compounds. The next type of organic molecules that one can encounter or one can think of are the carboxylic acid, where you have a C double bond O OH this kind of functional group called the carboxylic acid group. And these carboxylic acid groups are again at the terminal position. So we do not need to identity the position of it until and unless it is absolutely necessary. No need to mention the specific position of it.

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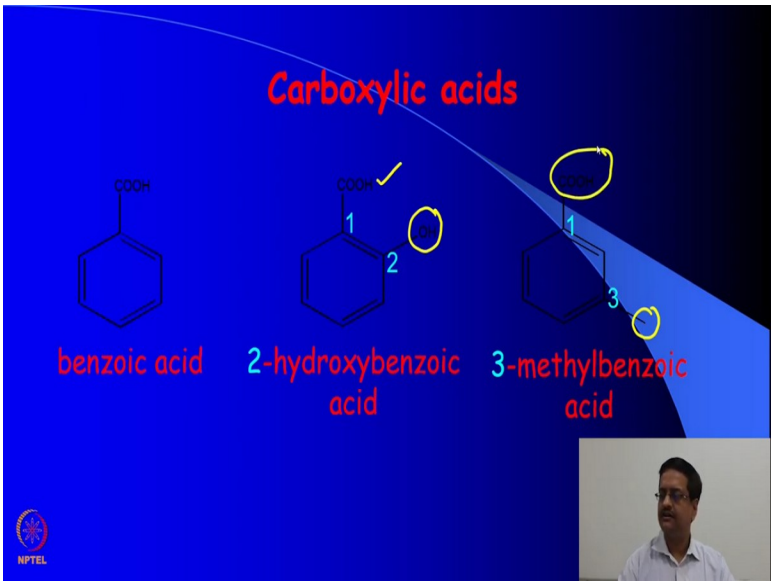

So in case of carboxylic acids containing aromatic rings so those are the benzoic acids when you have a substitution on benzoic acid we can write it as 2-hydroxybenzoic acid. You see here the

priority of carboxylic acid is given over the priority of OH group and then you can have 3-methylbenzoicacid. So the carboxylic acid gets higher priority over the methyl group.

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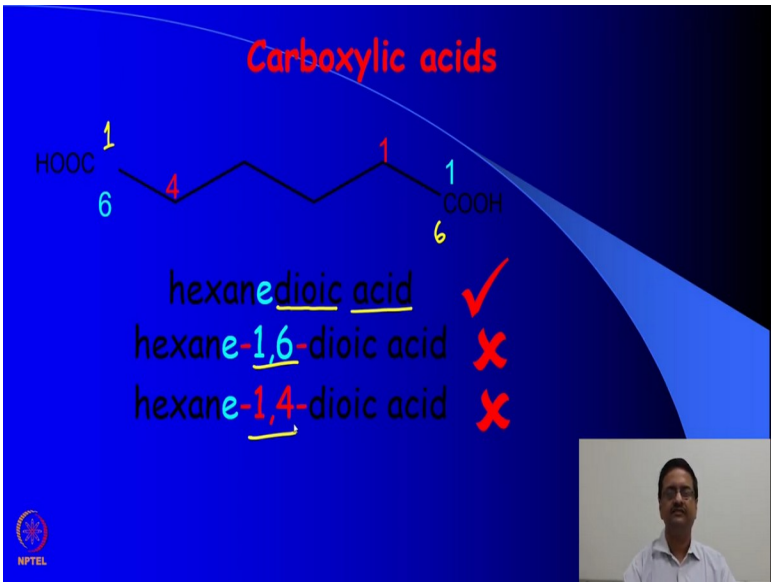

Now we have one example here we have a 6 carbon chain molecule. And we have carboxylic acid at either end. Depending on, how you identify whether you identify this as one and that end as 6 or this end as 1 and that end as 6 both are hexanedioic acid because there are dicarboxylic acid we write it as dioic acid. And we do not identify them as this position which I have already mentioned. So it will be hexane dioic acid not 1,6-hexanedioic acid.

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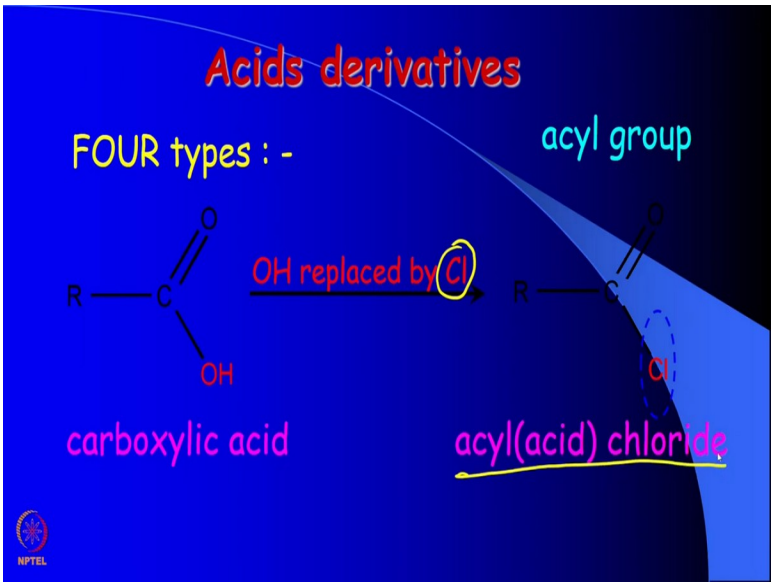

There are different acid derivatives. So when you have an acid and you replace the OH group by a chloride you get acyl chloride or acid chloride.

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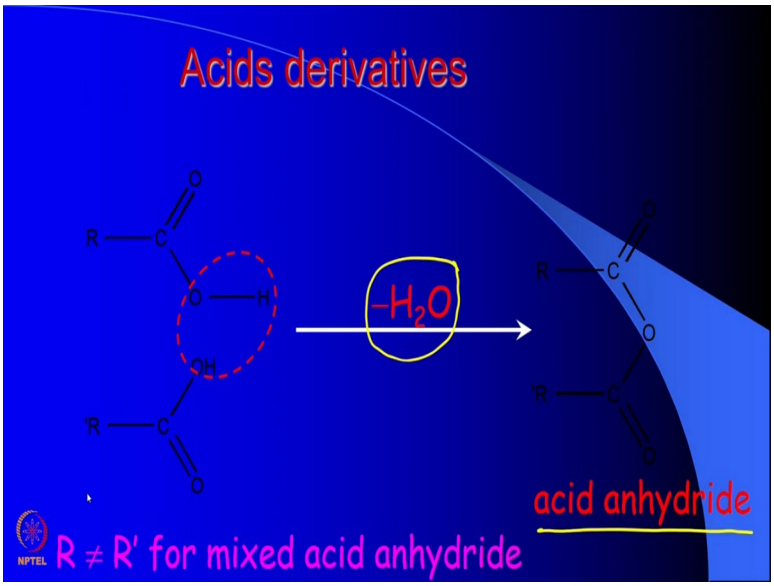

When you have 2 acid groups joined together by dehydration process and form a new type of molecule which is shown here this has R C O O C double bond O R kind of moeity that is called the acid anhydride. And it is possible that there may be R and R groups which are different and it forms a mixed anhydride.

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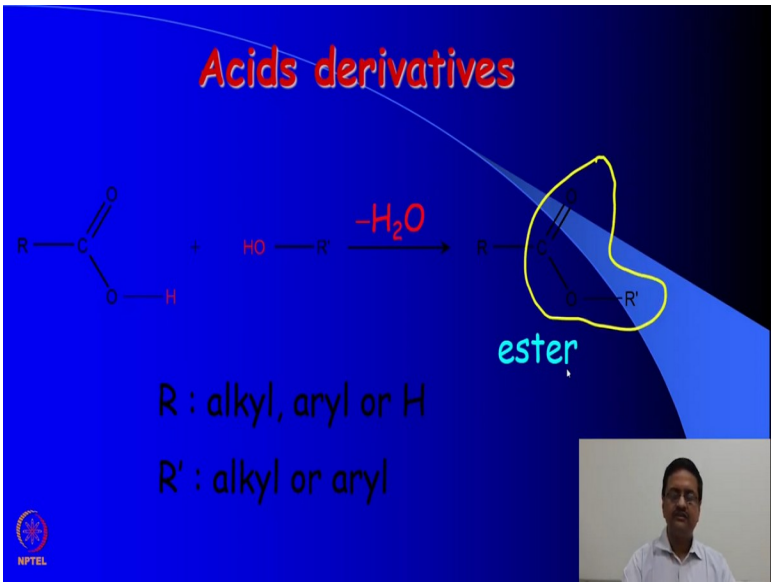

The next type of acid derivative is the reaction product of an acid with alcohol where it forms an ester that you can see on the right. This linkage is called the ester group which you may know that has a very nice fruity smell to identify an ester.

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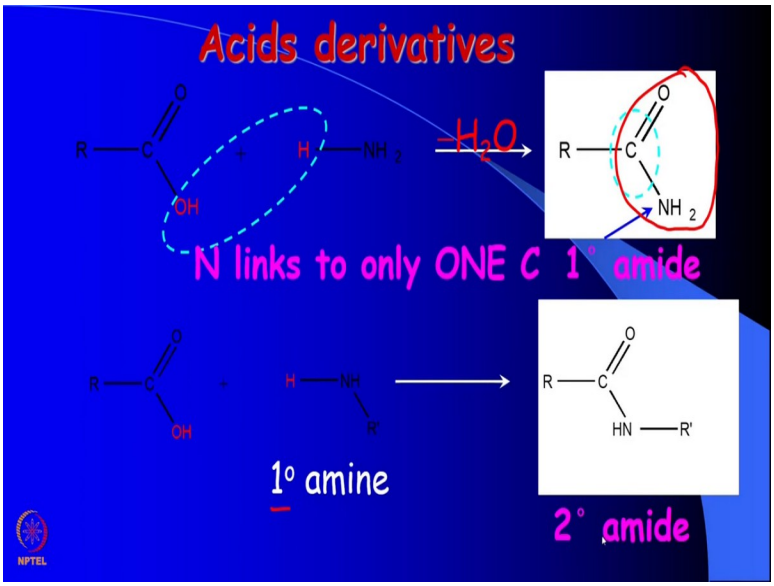

The other derivatives of acid can be amides. So when the acid is treated with amine it forms a CONH group as you can see on the right. So this is called the 1 degree amide and the other one is called the second or 2 degree amide. So when you have ammonia it form 1 degree amide when you have is an amine R-NH2 group then it is 1 degree amine forms a 2 degree amide.

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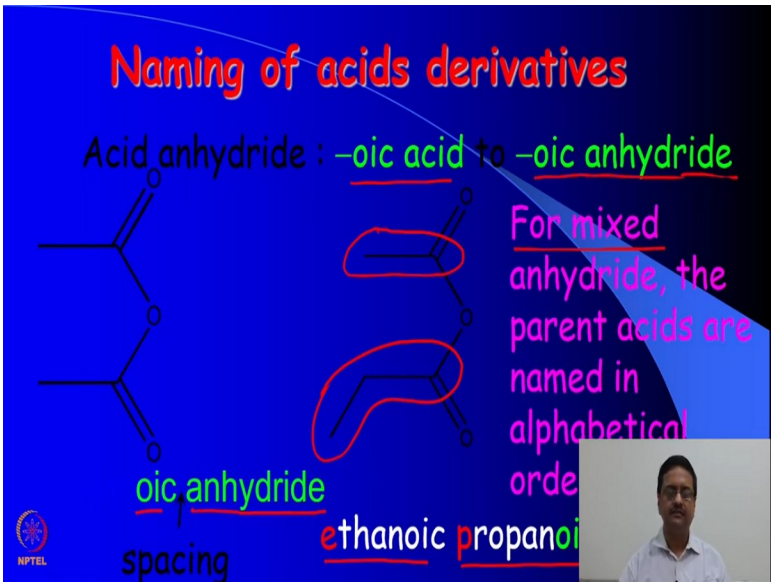

Let us now try to understand the naming of acid derivatives where we are trying to learn the how to name the acid anhydrides. So when you have a benzoic acid or carboxylic acid we write it as oic acid. So when that acid is converted to an anhydride we write it as oic anhydride. So you see there is a space between oic and anhydride. And as I, indicated in the previous slide that there may be a mixture of acids which can give you a different anhydride.

So when you have mixed anhydride the parent acids are named in alphabetical order. So the parent acid here is ethanoic acid. In this case the parent acid is propanoic acid. So the name that we identify for this type of molecule is ethanoic propanoic anhydride. So with this we would end this lecture and we will continue the discussion on nomenclature from here in the next lecture. Thank you.