**Symmetry, Stereochemistry and Applications**
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**Module No # 01**
**Lecture No # 04**
**Nomenclature of some complex molecules**

Welcome back to the course on symmetry stereochemistry and applications. In this lecture we will continue our discussion on the nomenclature of organic compounds. In the previous lecture we were discussing about the nomenclature of compounds derived from the carboxylic acid.

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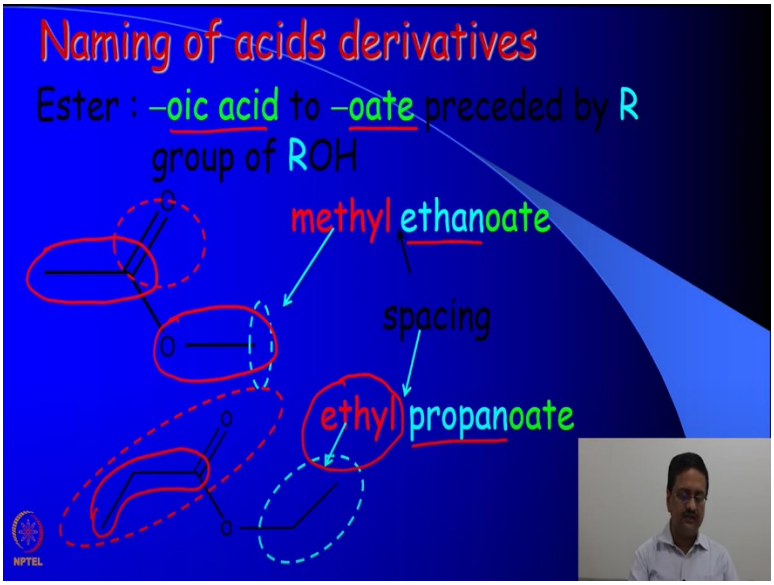


So here we will continue that discussion. So when you are trying to name the derivatives of carboxylic acids, as we all know that carboxylic acid are written as oic acids as you can see here. And when we convert that benzoic acid or any carboxylic acid to the corresponding ester we write it as oate. So carboxylic acid becomes carboxylate. So ethanoic acid becomes ethyl ethanoate or methyl ethanoate and things like that.

So in this case here in the example that I have written is that you have 1 carboxylic acid which is originating from an acid containing 2 carbons. So it was ethanoic acid. But then I have a methyl group which is connected to the oxygen. So then it is the methyl ester of ethanoic acid. So the name should be methyl ethanoate. Similarly when you have the next acid which is shown here has three carbon atoms.

So this one is originating from propanoic acid so it becomes, when it is ester the name becomes propanoate. And this signifies the corresponding ester part which has come from an alcohol which is ethyl alcohol. So from ethyl alcohol it has got generated so we write it as ethyl propanoate.

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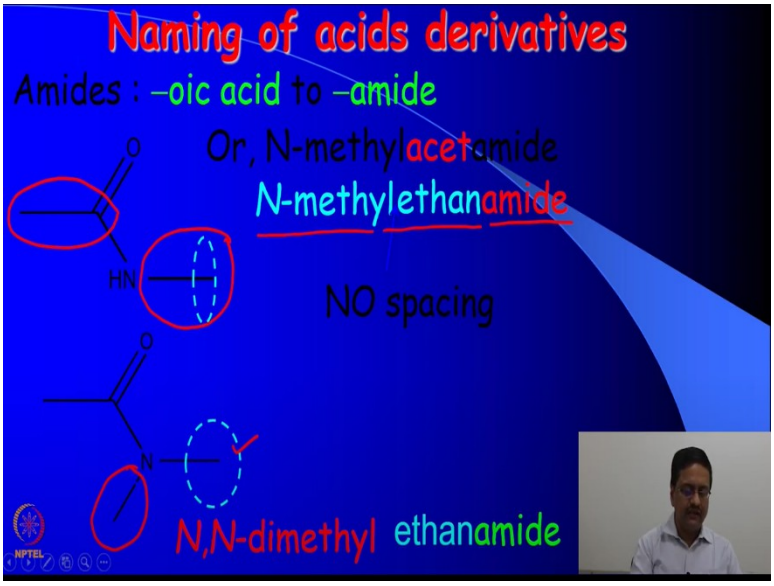


The next type of acid derivative is the amide which is also originated from benzoic acid or any organic acid. So with oic acid getting converted to amide we write the name as amide. So here in the first example once again it is originated from ethanoic acid. So we write it as ethanamide. And it depends what group is here. So depending on that it is N-methyl because at N, I have a methyl group present. So instead of methyl group if you had 2 methyl groups as you can see here we should write it as N, N-dimethylethanamide.

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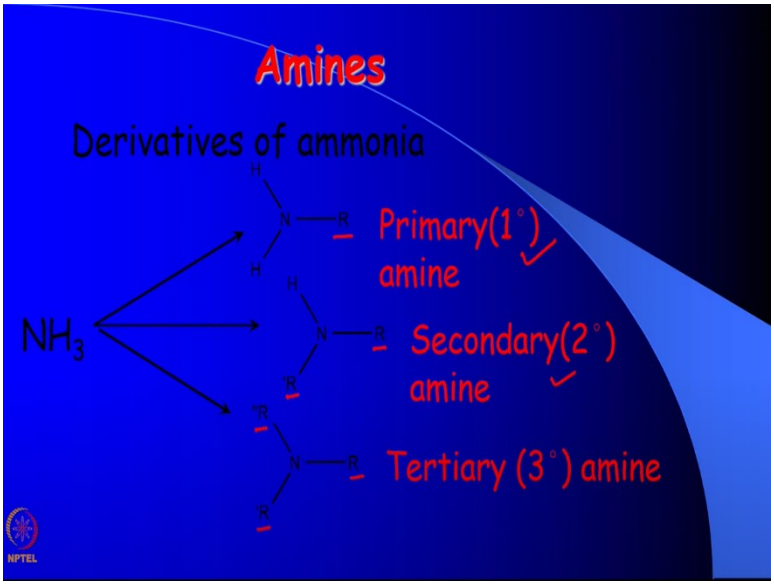


So this is how one should start naming the amides. So we have been talking about amines and amides and all that, in that discussion we have already discussed that there are possibilities of compounds called amines. So here I want to discuss quickly, what are amines? Amines are derivatives of ammonia. So from ammonia if you replace one hydrogen by an alkyl group it becomes a primary amine.

You replace 2 hydrogens with 2 alkyl groups then it becomes a secondary amine and the third hydrogen if you replace with the third alkyl group or aryl group it becomes a tertiary amine. So these 3 different types of amines responds to different types of tests which we will learn in different course.

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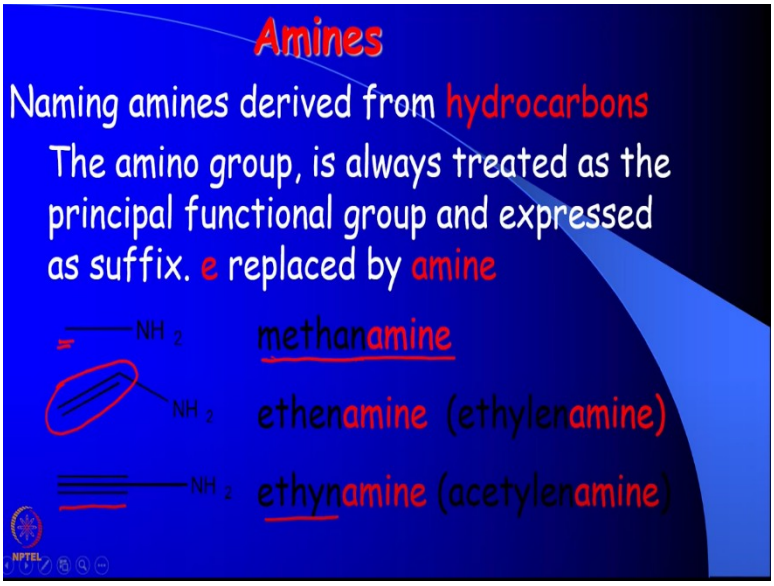


So when you talk about the amines the naming comes from the corresponding hydrocarbon. We first need to identify the long chain hydrocarbon from which it comes. And the amino group is always treated as the principal functional group and expressed as suffix. So here this e is replaced by amine. So for example, what are the names of 3 compounds. The first compound is coming from single carbon compound methane.

So instead of writing methan e amine we drop that particular e and written as methanamine. Similarly the next one is ethenamine or ethylenamine because this group is a double bond containing groups so ethenamine. And the third one as you could see that has a C triple bond C so it originates from the ethyne. So the last e is again dropped and amine is added at the end. So it is called ethynamine.

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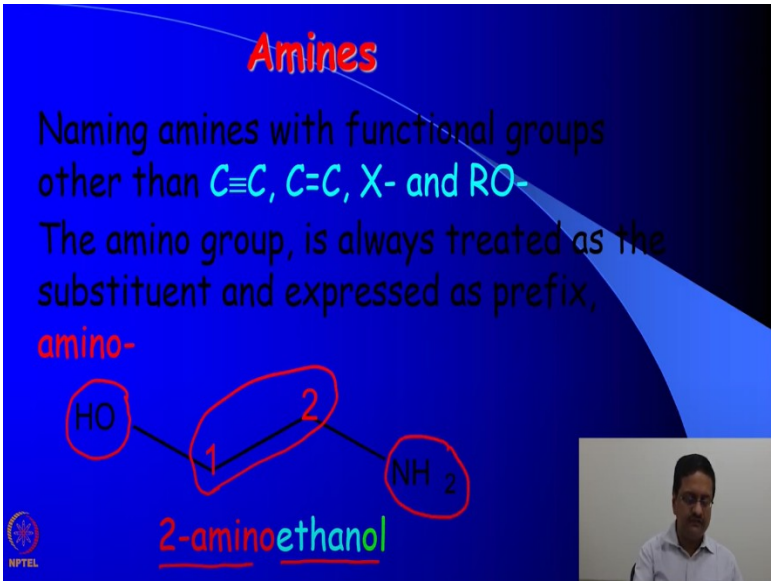


So when you have multiple functional groups we can name the amines with functional groups other than C triple bond C, C=C double bond, halogen and alkoxy groups. So the amino group is always treated as the substituent and expressed as a prefix. And amino it comes from when you have a molecule like that which has 2 functional group at two end OH and NH2. OH has a higher priority so the compound is ethanol where this part signifies the ethane, this part talks about ol. And at 2, position you have the amine group. So we write it as 2-aminoethanol.

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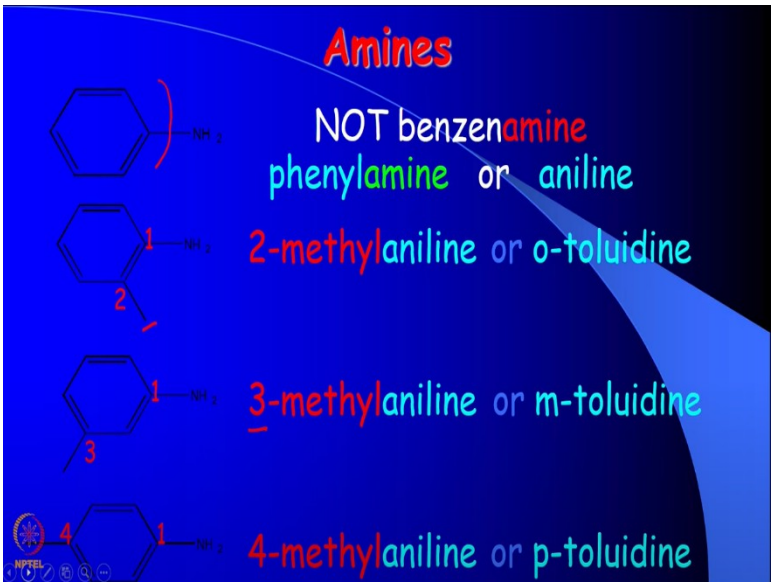


There are possibilities of aromatic amines. So here we do not write as benzenamine rather we write phenylamine because the group which is C6H5 is the phenyl group, we have a specific name for that called aniline. Similarly when you have multiple substitutions you start numbering

them following the same method that we have discussed in the previous lectures and apply the numbers and then write the corresponding names.

So in the first case it is 2-methylaniline, second case it is 3-methylaniline and the fourth case it is 4-methylaniline. These are the common names of those three compounds those are respectively ortho toluidine, meta toluidine, and para toluidine.

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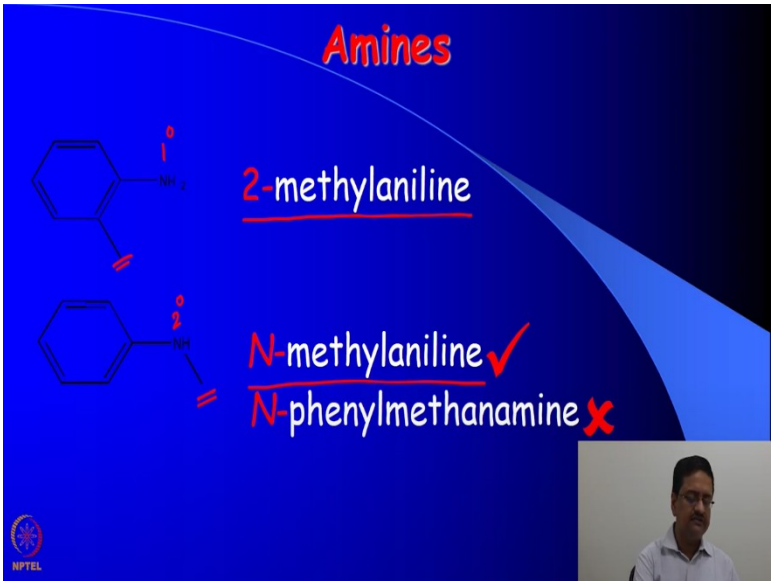


Now you see the difference. These 2 compounds which are drawn on the left hand side have the same molecular formula but the position of methyl group is different. So in the first case the methyl group is connected to the aromatic ring. So it is named as 2 methylaniline and this nitrogen is 1 degree that is it is a primary amine. But when the methyl group is now connected to that nitrogen we write it as N-methylaniline and that N, the nitrogen here is a secondary nitrogen that means this N-methylaniline is a secondary amine.

In this case we should not write as N-phenylmethanamine because this ring is the major ring which is the phenyl ring.

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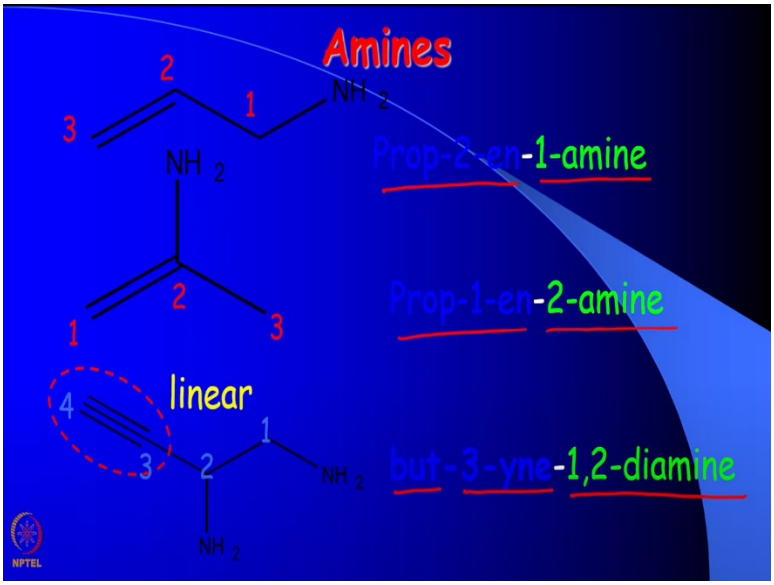


So what would be the names of these 3 amines. We should start numbering them as usual. So we should number in such a way that amine gets the lowest priority over double bond. And then try to write the name, In this case it is 1-amine because at 1 position it is NH2 and the compound is derived from propane and there is propene and there is a C=C double bond between 2 and 3 we write is as prop-2-en-1-amine.

The second compound is named as prop-1-en-2-amine. Why? Because now if you try to number it in any direction from left to right or right to left NH group always appears at number 2. But now if you write it from left to right the en comes at number 1 position. Therefore it should be written as prop-1-en 2-amine. And the third one you see here what we have is a 4 membered chain 1, 2, 3 and 4.

So we have 2 amino groups so it must be diamine we write it as 1, 2-diamine. And this being a derivative of butane rather butyne we have C C triple bond. So we write it as 3 yne. So the name directly simplifies the particular molecule which is shown here.

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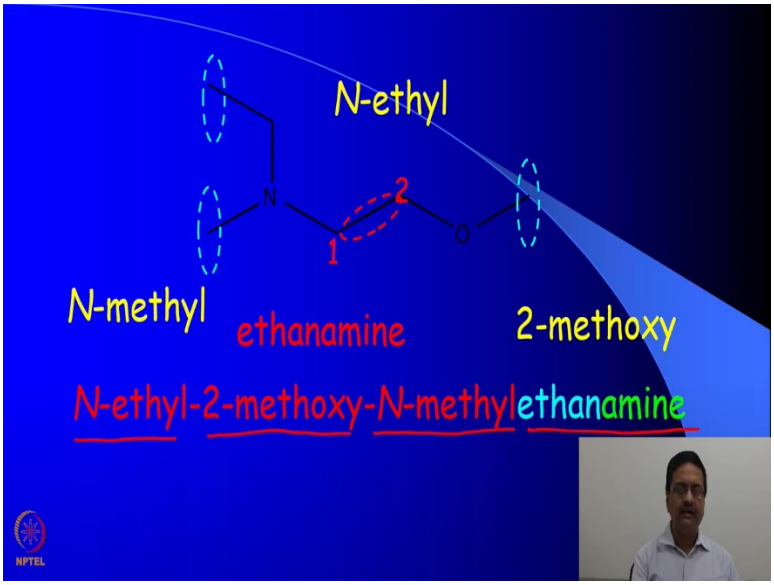


Now let us see how do we name this kind of a molecule. What can we see in this molecule? We have C-C single bond in the middle, in this red circle. So on that we have a nitrogen. So it is called ethanamine. Then what we have is on this nitrogen we have ethyl group and then there is a methoxy group and also there is another N methyl group. So what should be the name of this compound? The name of this compound should be N-ethyl-2-methoxy-N-methylethanamine.

Now you see here what we are trying to follow is the alphabetical order of those substitutions ethyl, methoxy and methyl once again. So this one has to remember that after identifying the longest chain you should find out the substitutions and once you are sure about the substitutions then try to write those substitutions in the alphabetical manner to get the name of the compound.

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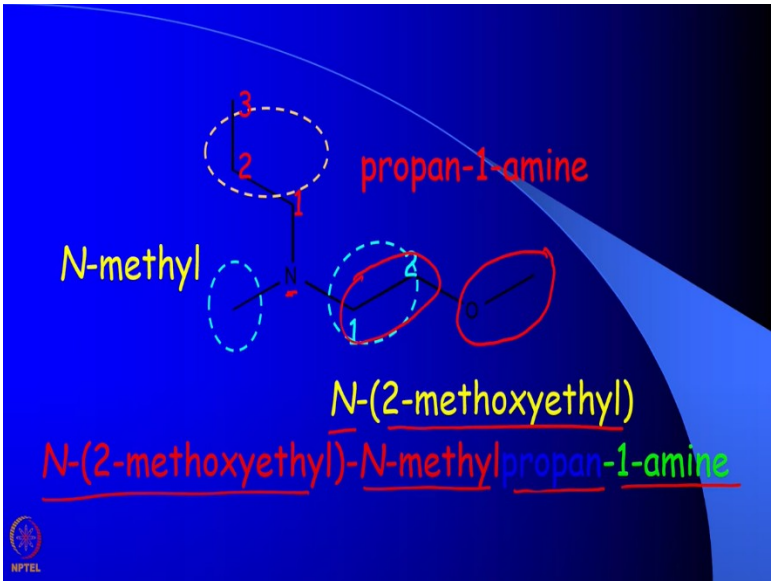
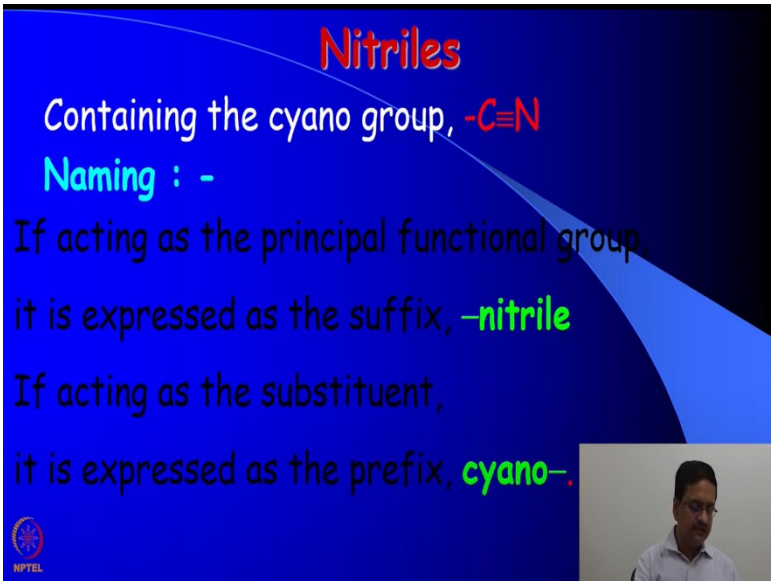



So applying the same logic what should be the name of this compound. If we carefully see that the longest chain is now different. It is not the central C-C bond which was the earlier case but in this case the side chain with 3 carbon atom is the longest chain. So it is a derivative of propan-1-amine. What we have is 1, 2 that is ethane. So what we should write is that the nitrogen is attached to a 2-methoxyethyl this is methoxy group, connected to 2 position. So it is 2-methoxy ethyl that is connected to nitrogen.

And then we have N methyl substitution on the left. So, all together the name should be N-(2-methoxyethyl)-N-methylpropane-1-amine. So once again you see here we are following the rules that we have learnt from the very first class. We need to identify the longest chain. We need to identify the substituents and then write the name with the alphabetization of the substitutions. **(Refer Slide Time: 14:05)**




The next sets of molecules are called the nitriles which contains a C triple bond N group. This can be of 2 types. If it is acting as a principle functional group it is expressed as the suffix nitrile. And if it is acting as a substituent it is expressed as a prefix cyano. So let us see these 2 cases one after another. So here we have 2 compounds which are written as ethanenitrile and 2-methylpropanenitrile because in both the cases the cyano group is the only substitution or only functional group.

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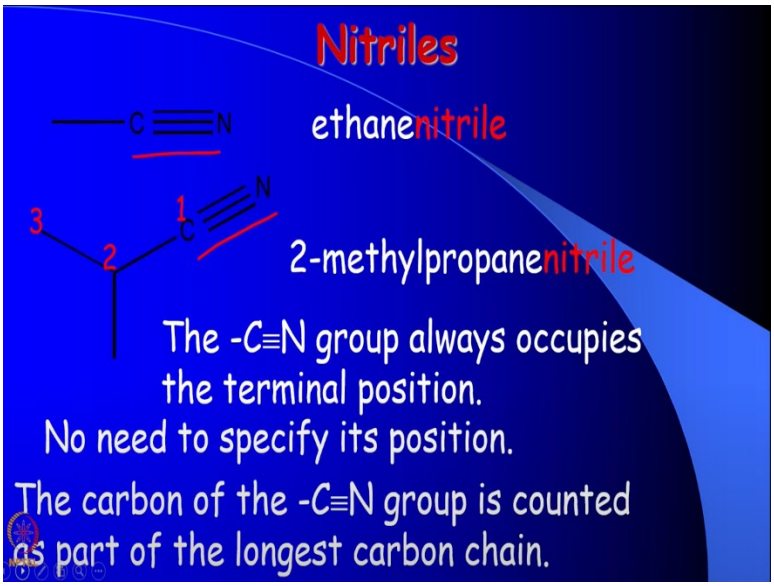


The carbon of the CN group is counted as the part of the longest carbon chain in these two cases. And the CN group always occupies the terminal position just like the condition with aldehyde or carboxylic acid. So we do not need to mention the position of this particular CN group.

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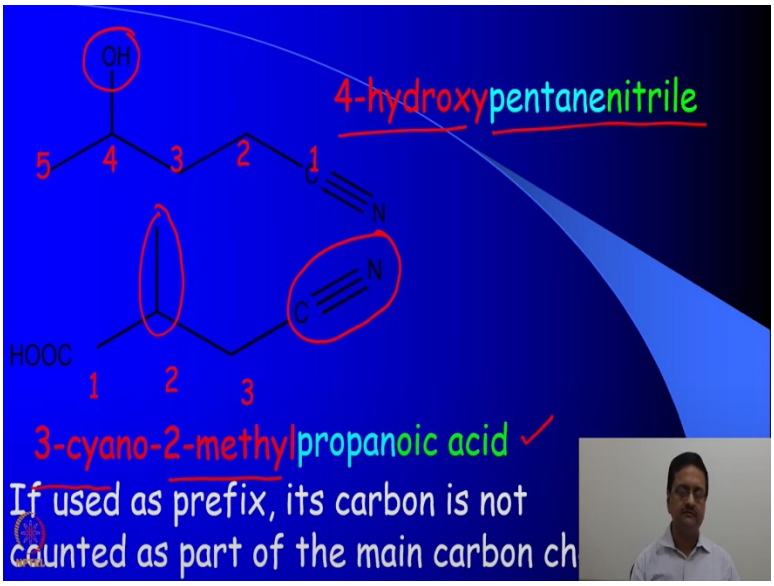


But now when, we have molecules like this where you have hydroxyl group and cyanide or carboxylic acid with cyanide group. So we first name them number them find the longest chain and apply the numbers and then try to write the name. So in this case the first case you have hydroxyl group at position 4. So we write it as 4-hydroxypentanenitrite. In the second case we write this numbers as 1 2 and 3 and do not count that fourth one.

And write is as propanoic acid that is the beginning and then we have a methyl substitution at 2 position and cyano substitution at 3 position. So we write the total name as 3-cyano-2-methylpropanoic acid. So here you can see the priority of cyanide is lower than the priority of carboxylic acid. So in those cases the cyanide group is written as cyano not as nitrile. But when the cyanide group is the principle group we write it as nitrile. So, if used as a prefix its carbon is not counted as a part of the main carbon chain which is done here.

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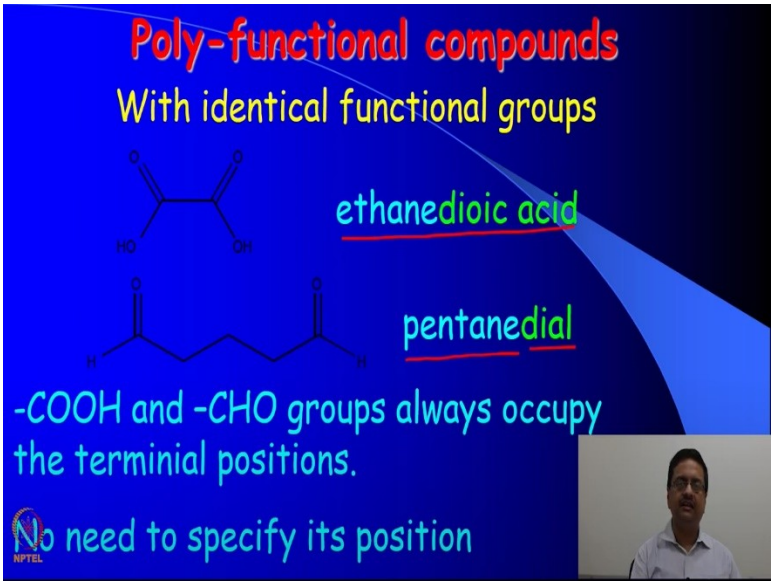


There are many organic compounds which has more than 1 functional groups may be same or different. So they should be named in that way. So here we have a dicarboxylic acid which is commonly known as oxalic acid, its IUPAC name would be ethanedioic acid. The second compound has 5 carbon chain at that 5 carbon chain is already named as pentane and we have 2 aldehyde groups at 2 terminals. So we write it as pentanedial.

CO2H and CHO groups always occupy the terminal position which is always to be remembered. So we do not need to specify their position when we are trying to write their names.

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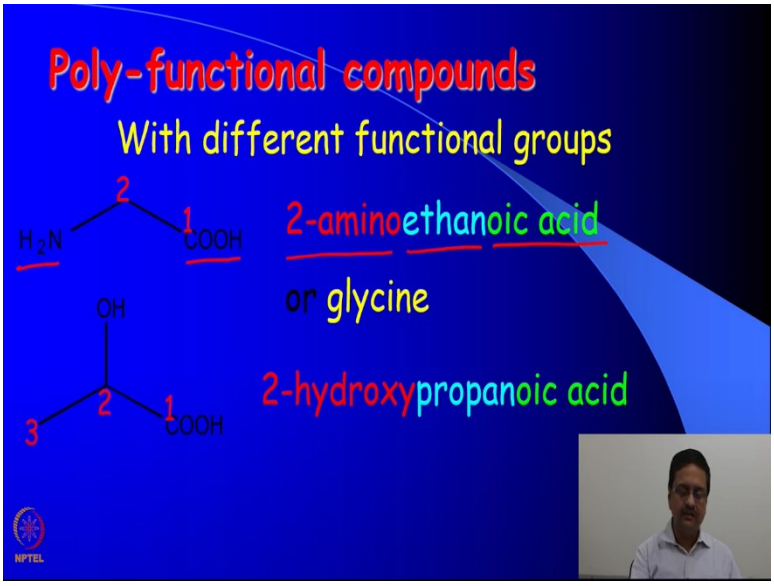

So when we have poly-functional compound with different functional group we need to prioritize them and we need to write them as per their class. So here the first case is a carboxylic acid with amine. So the carboxylic acid is written as oic acid. It is originating from ethane so it is ethanoic acid. And then you have the amino group present which is a two amino substitution. So the name appears as 2-aminoethanoic acid or the common name is glycine. The second one is 2 hydroxypropanoic acid. Again here the acid is a 3 membered chain. So it is propanoic acid and the substitution is to 2 hydroxy.

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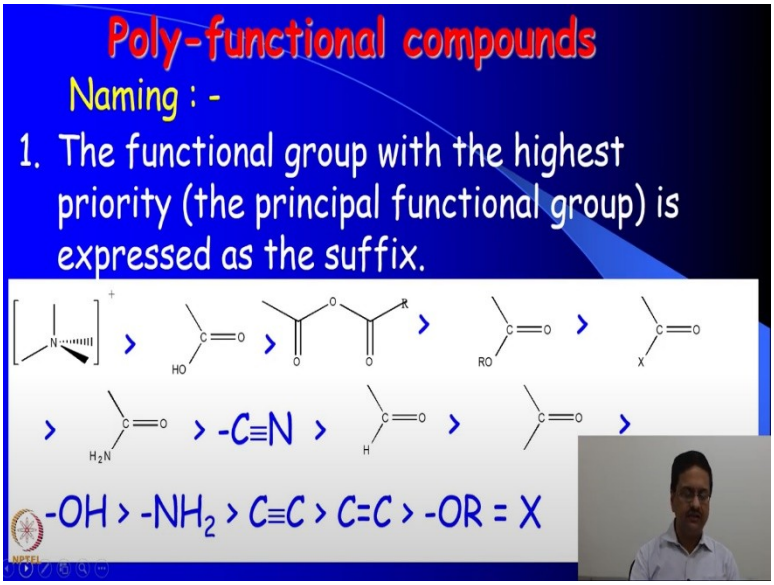


So when we try to write the priority order for different functional groups we need to remember this particular flow that which comes above what? So I would like you all of you to pay attention to this chart and remember their priority and based on this priority the names of those organic compounds will be determined. In the next few minutes, we will try to understand the bicyclic compounds, the nomenclature of these compounds.

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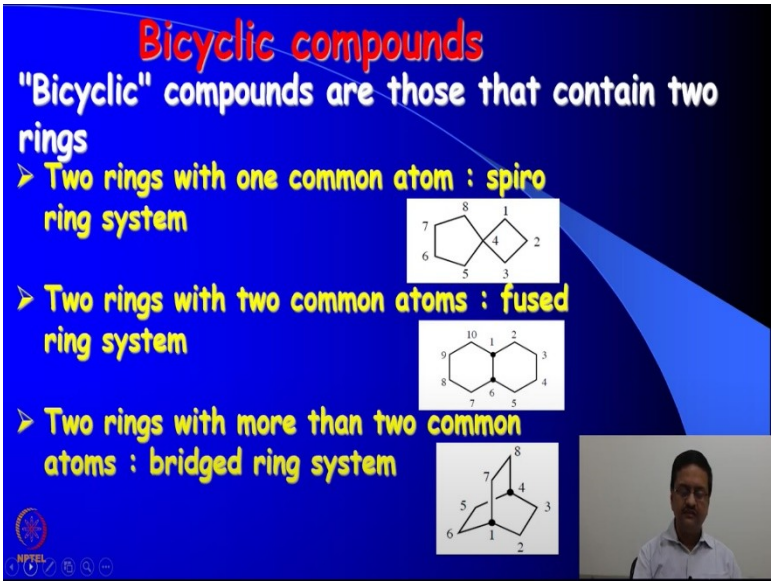


Bicyclic compounds are those that contain 2 rings. There are 3 different types of bicyclic compounds. 2 rings with one common atom is spiro system which is example here. 2 rings with 2 common atoms and those 2 common atoms are connected together called the fused ring system. This is one such example. And 2 rings with more than 2 common atom and the common atoms are not connected they are called the bridge systems. So this is called that the bridge system that you have here.

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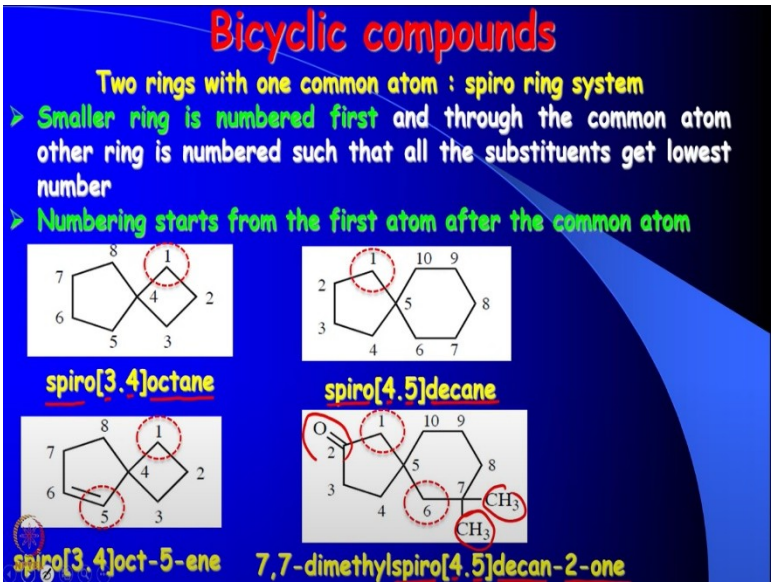


So when we try to name these bicyclic compounds these 3 different types need to be addressed in a different way. In case of the first type spiro ring system this smaller ring is numbered first and then through the common atom the other ring is numbered in such a way that all the substituents

gets lower priority. So you write it as 1, 2, 3, 4, 5, 6, 7, 8 the number of atoms present in this smaller ring and the number of atoms present in the bigger ring and these has 8 carbon atoms. So it is octane.

So we write it as spiro[3.4]octane. The second one here that we have is numbered like that 1, 2, 3, 4, 5, 6, 7, 8, 9 and 10. So this is a derivative of decane it is a spiro compound. And then on the left hand side ring you have 4 carbon atoms. And the right hand side has 5 carbon atoms. So let us talk about the fourth example, the third one I am leaving for you to understand yourself. The fourth example I am numbering in this way 1, 2, 3, 4, 5, 6, 7, 8, 9, 10.

Here you see the numbering has done is such a way that this functional group here gets the lowest number. Here the substitution also gets the lowest number. So this becomes decan-2-one because you have ketone at 2 position. And then it is a spiro compound and there are 1, 2, 3, 4 atoms on the left side ring and 5 atoms in the right side ring so 4.5. And the dimethyl appears at 7 position. So we write it as 7, 7-dimethylspriro [4.5]decan-2-one. These numbers are represented in square brackets. So always we start the numbering from the first atom after the common atom.

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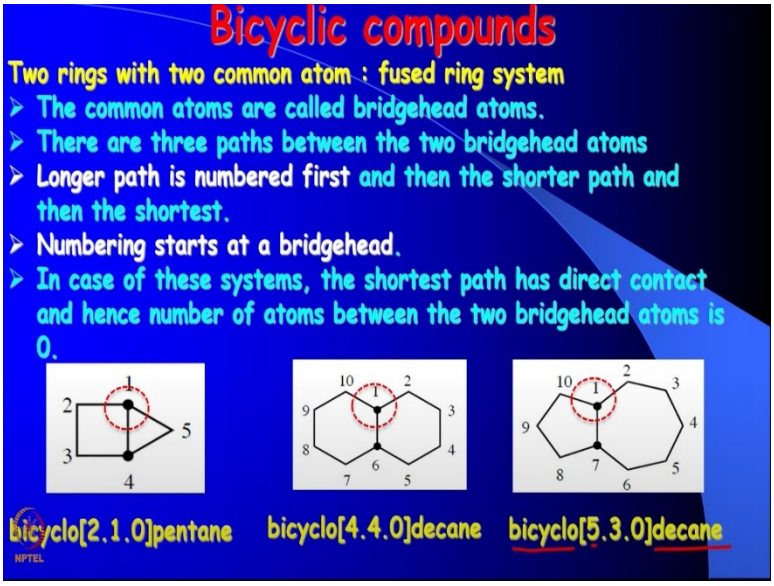


So when we come to then next type, which is fused ring systems there are common atom that are called bridged atoms. There are 3 paths between the 2 bridged atoms. Longer path is number first and then the shorter path and then the shortest. And always the numbering start at bridgehead. In

case of this system the shorted path has direct contact and hence the number of atoms between them, that is the 2 bridgehead atoms is 0.

So the way we write the name is shown here. In the first case we write it as 1, 2, 3, 4 and then 5. So there are 2 atoms between 1 and 4 on this side. There is one atom between 1 and 4 on that side and 1 and 4 are directly connected. So we write it as bicylco[2.1.0]pentane. Similarly the last one that you have here is numbered as 1, 2, 3, 4, 5, 6, 7 so the largest ring is numbered first.

And then goes the other side 8, 9, 10. So it is written as bicyclo decane and these numbers 5 is the number of atoms in the largest ring then the number of atoms in the smaller ring and 0 indicates that these 2 atoms are bonded together.

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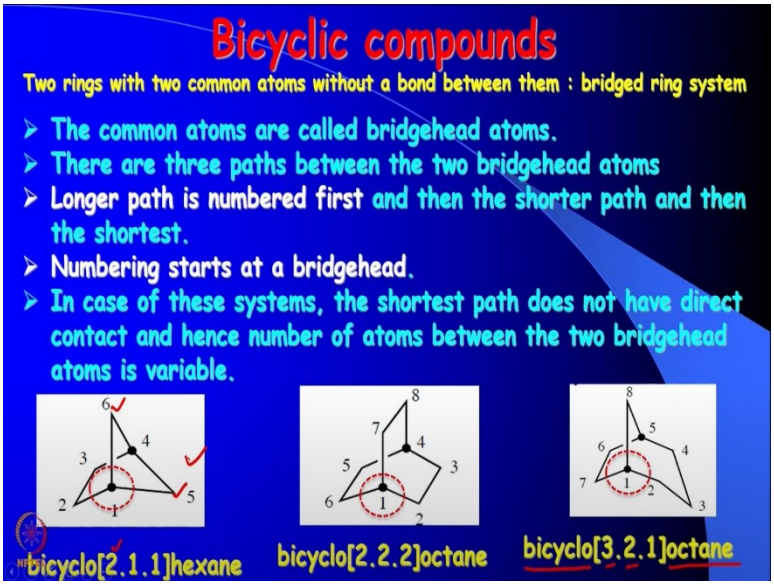


The third type of bicyclic compound is the bridged ring system. So here the common atoms are called bridgehead atoms. There are 3 parts between the 2 bridgehead atoms. The longest path is numbered first and then the shorter path and then the shortest path. The numbering starts at bridgehead. So in case of this system the shortest path does not have direct contact and hence the number of atom between the 2 bridgehead atoms is variable. So here when you try to write these names we should again write it as bicyclo and hexane.

As you can see there are 6 atoms here in this particular molecule. And we have 2 atoms on that ring so it is 2. One atom here between these 2 on that ring it is 1 and 1 atom there it is 1. So in

the same manner the third one here we can see that it has 2 bridgehead atoms we start numbering from one of them. Number 8 in the longest ring first and then the shorter ring. And then we write it as octane because there are eight carbon atoms.

And then from 1 to 5 we have three atoms here. From 1 to 5 from that side you have 2 atoms and from 1 to 5 through 8 we have one atom. So we write it as bicycle[3.2.1]octane. This is how you should number these bicyclic compounds.

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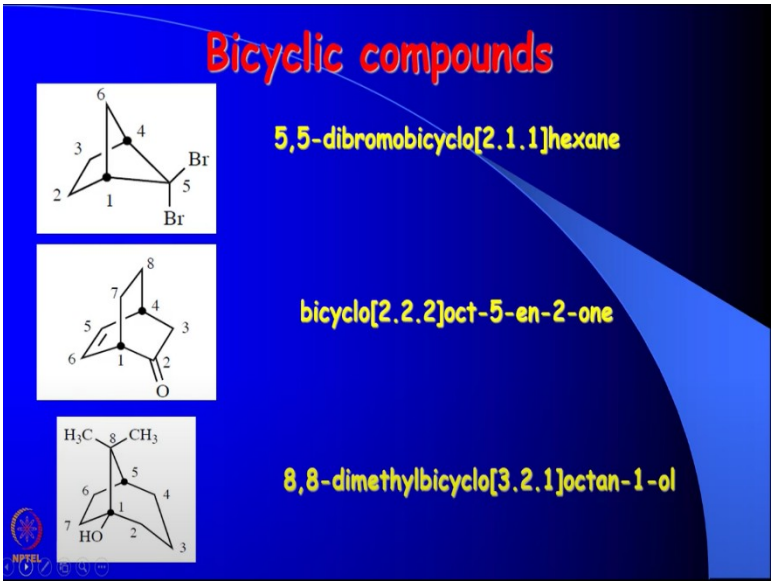


These are some other examples of bicyclic compounds that you may want to learn yourself how these naming are done.

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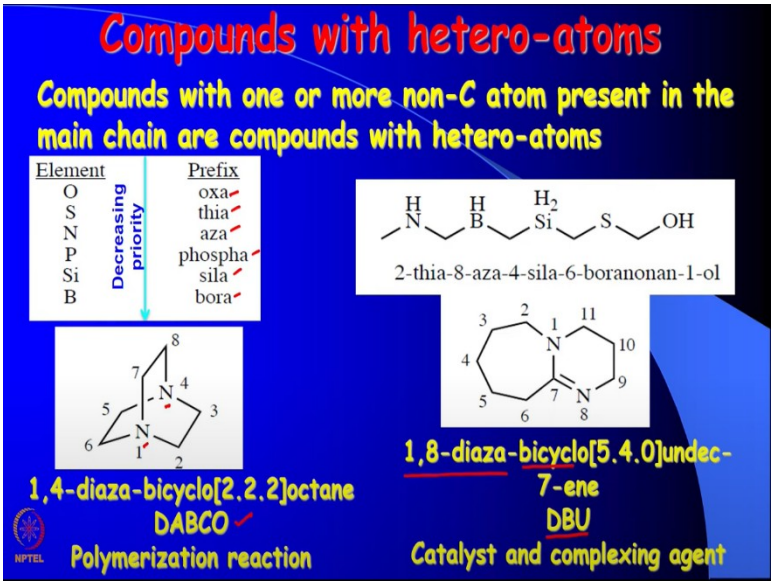

The last type of compounds that I would like to touch on are the compounds which contain atoms other than carbon, hydrogen, nitrogen, oxygen see for example boron, silicon, phosphorous etc., So when you have this kind of substitutions we have different prefixes for different elements.

And here is one example which is a very well know compound that DABCO used in polymerization reaction. This is nothing but the bicyclic compound containing the hetero atoms. So we write it as bicycle[2.2.2]octane if it was just carbon. But then at 1 and 4 you have nitrogen so we write it as 1,4-diaza-bicyclo[2.2.2]octane. Similarly DBU is another compound which is used as a catalyst and complexing agent.

And this compound falls as another bicyclic compound where the 2 common atoms are joined together joined by a bond. So the name is similar bicycle[5.4.0]octane because this side you have 5 atoms, on the other side you have 4 atoms. And the bonds is there between the 2 atom. So it is bicycle[5.4.0]undec-7-ene because you have double bond at 7 position. And there are 2 aza group so we write it as diaza; 1, 8 diaza. So like this we can name all kind of molecules that we may encounter in this course.

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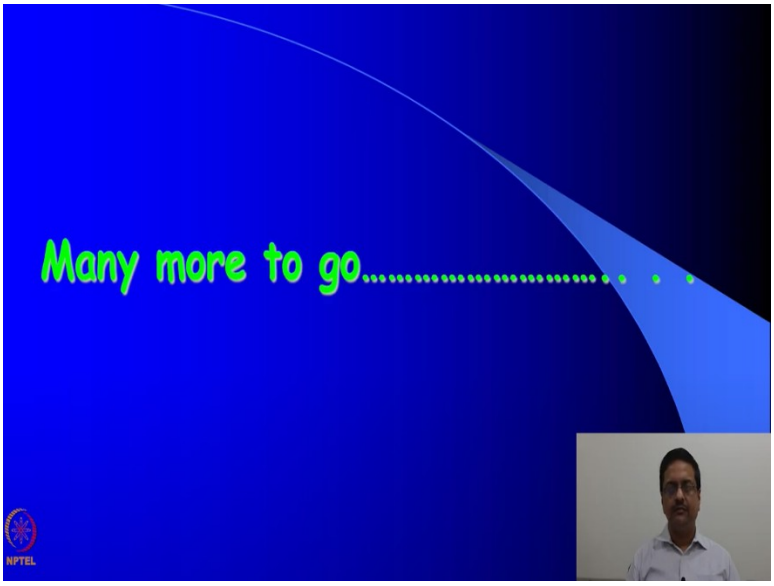


So with this I would like to end the part of this course where we talked about the IUPAC nomenclature of organic compounds.