Symmetry, Stereochemistry and Applications
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Module No # 01
Lecture No # 05
Practising Naming of Molecules

Welcome back to the course entitled symmetry, stereochemistry and applications. In the first 4 lectures in this course we have discussed about the rules of IUPAC nomenclature. And I have described almost all the rules that one need to know and then start writing the names of different organic compounds. So in today's lecture we will take a few examples and we will try to apply our understanding of IUPAC nomenclature for some simple organic molecules.

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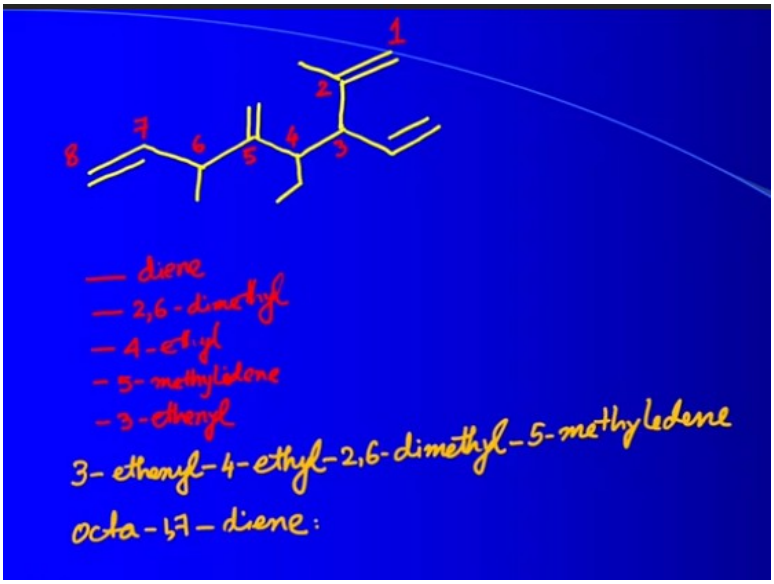

So let me draw the first molecule on board. Along with me you should also draw the molecules using your pen and paper so that you can understand it better. So what are the functional groups that we are seeing in this particular molecule? We are seeing a few double bonds and there are some alkyl substitutions. So the first point in this case would be to identify the longest chain and we should identify the longest chain in such a way that the double bond gets the lowest numbering and you have the maximum number of branches.

And in addition what you should have is the branches or the substitution should have the lowest numbering as well. So considering all that points you will understand very easily that the

numbering should start from this carbon atom at the top right hand corner. So we should number it like 1, 2, 3, 4, 5, 6, 7 and 8. So when you find that this molecule has 8 carbon atoms and in the main chain from 1 to 8 there are 2 double bonds.

So by nature this is a diene so the last part of it would be diene. Then we need to find out what are the various substitutions that are present. So what we see here we have methyl groups at 2 and 6 positions so, we should write that as 2, 6-dimethyl. And then at 4 position we have ethyl and then at position 5 we have methylidene and then what we have is at 3 position we have ethenyl. So what should be the name of this molecule? We need to alphabetize these substitutions and write the name accordingly.

So when we try to write the name we should write it as I am writing here 3-ethynl-4-ethyl-2,6-dimethyl-5-methyledeneocta-1,7-diene. Hope you are able to follow this nomenclature. Now I would like to draw a different molecule where we have a cyclic ring system present in the molecule.

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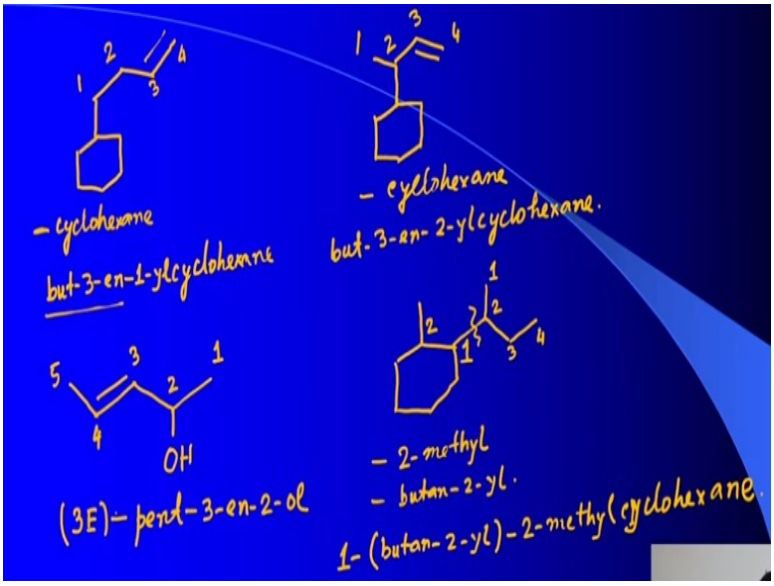

So what we have is a cyclohexane moiety along with that I have a slightly long side chain like that, a second molecule of similar type as I am drawing here as a slightly different connectivity. What are the names of these 2 molecules? So in the first case what we have a cyclohexane that is the main compound and we have a side chain which as 3 carbon atoms, sorry I have not drawn it right.

So this as 4 carbon atom connected so this is a group of butane or rather butene and what we have at 3 positions is en. So it is 3-butene so, what are name should be we should have the butene written as but-3-en and this but-3-en is connected to the cyclohexane ring through the atom 1. So it should be 1-yl cyclohexane. See the nomenclature what we have done here we have first found out the cyclic chain and numbered the side chain in such a way that the connectivity of that side chain with the cyclohexane ring gets the lower numbering.

And then we have written the name of that side chain as this. So using the same method for the next molecule again we have it as a cyclohexane. And a butene but the connectivity is different so if we write it like that 1, 2, 3 and 4 the connectivity is through the carbon number 2 so you can easily understand that the name of this compound should be but-3-en-2-ylcyclohexane. So this is how one should number a cyclic compound with a complicated chain outside the molecule.

Then let us try to draw a different molecule where we will have a double bond and also an hydroxyl group present in that. So what should be the name of this compound? We should start numbering in such a way that hydroxyl group which is a higher priority group should get the lower numbering. We should start numbering this molecule from the right hand side such that the oxygen gets the priority, the atom number 2, 3, 4 and 5.

So this is a derivative of pentane and it has OH group so it is pentane-2-ol and then you have a en that is double bonded 3 position and that double bonded 3 position is nothing but E which means it is trans. So we should write it as (3E)-pent-3-en-2-ol so it is 3 pentenol or pent-3-en-2-ol with 3E that is that signifies the geometry across the double bond. And then we try to name another molecule which is similar to the previous 2 but it has 2 different substitutions.

1 methyl group and second one as a side chain like that which is a butane or butyl group. So what we should do here? This is a cyclohexane but then we need to identify the carbon atoms of cyclohexane by numbering because there are more than 1 substitution on the cyclohexane ring. So the carbon containing a larger group gets number 1 and the second group gets number 2 so what we have is a 2-methyl and what we have is butane and 1-butyl group where you should number that chain as 1, 2, 3, 4 and the connectivity is through the carbon number 2.

So it should be written as butan-2-yl, so therefore the name of the compound should be at position number 1, I have butane-2-yl-2-methyl cyclohexane. So this is how one should logically follow the rules that we have learnt in the first couple of classes and try to write the names of different organic compounds. Now look at the next set of molecules which are very interesting because they all looks very similar but their numbering schemes are going to be slightly different.

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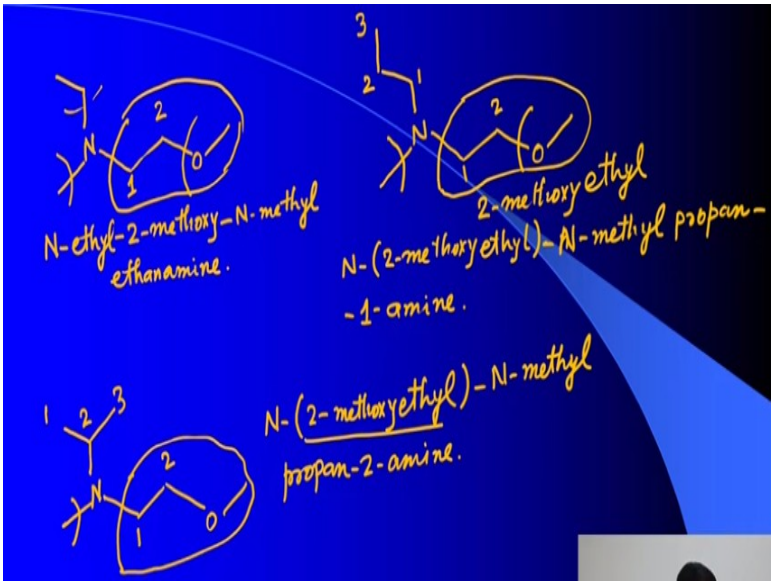

So the first molecule that I am drawing is like this, the second molecule that I want to draw is the following. And the third molecule that I should try to draw is this one. So what we see here in the first molecule among these 3 we have this ethane moiety which can be numbered as 1 and 2. And then here on the 2 position we have a methoxy group, on nitrogen we have ethyl and 1 methyl substitution.

So the name of the molecule should be N-ethyl-2-methoxy-N-methylethanamine. In the second case on the right hand side we have inside a 2 carbon chain. And here there is a 3 carbon chain, this 3 carbon chain gets priority and that makes this as propane amine instead of ethanamine and we have this group as a substitution on nitrogen and that group as a substitution on nitrogen. So we write the name of this group as 2-methoxyethyl this group is methyl.

So what we should write the name as N-(2-methoxyethyl)-N-methylpropan-1-amine. So what we have is here we have 3 substitutions getting priority over 2 substitutions. The third molecule of

this series is similar to the second molecule, here also in the middle we have 2 carbon atom chain but on the nitrogen I have a 3 carbon atom chain. So this is again a propanamine but not like the previous one when it is propan-1-amine it is propan-2-amine and this group remains as it is.

And I have N methyl as it is, so the name of this molecule should be N-(2-methoxyethyl)-N–methylpropan-2-amine. So you see depending on the molecule and their are number of carbon atoms we need to identify which is the parent molecule and based on that parent molecule we need to identify which one is a substitution and then we write the name of the substitutions correctly the way we are writing here and then we write the name.

If you look at these 3 molecules, all the 3 molecules have a group like that, but the way we write the name of that group in this 3 cases is different. In the first case we write it as a methoxy group because the other 2 carbon atom forms the parent chain. In the second and third example, the entire group is a substitution on nitrogen and the parent chain is something else. So one as to really look at the molecule and try to identify which is the parent chain and which is the substitution on a parent chain.

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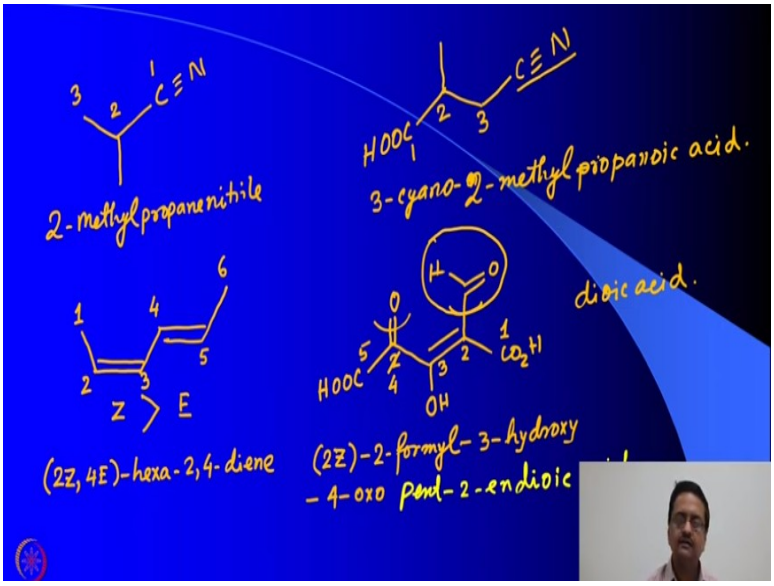

Now let us draw 2 more examples containing cyanide group. So what is the difference? In 1 molecule you have only 1 functional group that is the CN or this cyanide group. In the other molecule you have 2 functional groups so one is carboxylic acid and the other one is cyanide. So in the first case we should write it as, the numbering should be 1, 2 and 3 and write it as 2-

methylpropanenitrile. Because here this cyanide is the only functional group we write it as nitrile.

On the other hand for the second molecule we should number it as 1, 2 and 3 leaving the carbon connected to cyanide as substitution and the name of that molecule then should be 3-cyano-2-methylpropanoic acid. So when cyanide is not the only functional group or the main functional group we write it as cyano and when it is the only functional group or the main functional group we write it as nitrile.

Now we again go back to a simple molecule which is essentially a diene but here I would like you to see that the 2 double bonds that are drawn one of them is E and the other one is Z. So this double bond is in the Z configuration and that double bond is the E configuration. So which one should get priority and from which side we should number the atom. Of course Z gets priority over E so as a result we number the atoms from the left hand side.

So what should be the name? The name of the molecule should be, first we should identify the stereochemistry about the double bond so it is (2Z, 4E)-hexa-2,4-diene. So here what we learnt is that the Z being higher priority, the numbering starts from the side where Z comes first. Now we try to see what happens when you have combination of carboxylic acid, alcohol, some double bond and an aldehyde present altogether in a molecule.

So I am trying to write the molecule which is complicated so what we have is acid, a ketone, one alcohol, this is connected to a double bond and then you have a C double bond O H, CO2H. So by looking at the molecule you can directly identify that this is a di-carboxylic acid. So it should be written as dioic acid at the end so that is family of the compound. But then the numbering should start from the side where you have the higher priority groups.

So from the right hand side we have at position number 2 we have this group and from left hand side at point number 2 we have group, which is oxo. So what we should write is this group being a larger group we identify the numbering from the right hand side and write the numbers 1, 2, 3, 4 and 5. So this becomes pentanedioic acid and now we should try to write down the name. What is the configuration at 2, the 2 has the double bond which is in the Z confirmation.

So we should first write the configuration of the double bond as 2Z then we try to write the name of the compound as on 2 position this group being the aldehyde group as a substitution we should write it as a formyl group. So it is 2-formyl, at 3 position we have hydroxy, at 4 position we have oxo, then we have pent-2-endioic acid. So this is the name of the compound when you have many functional groups which are significant here like OH, aldehyde and oxo. So with this I would like to give you some homework so that you can try to name some of these molecules.

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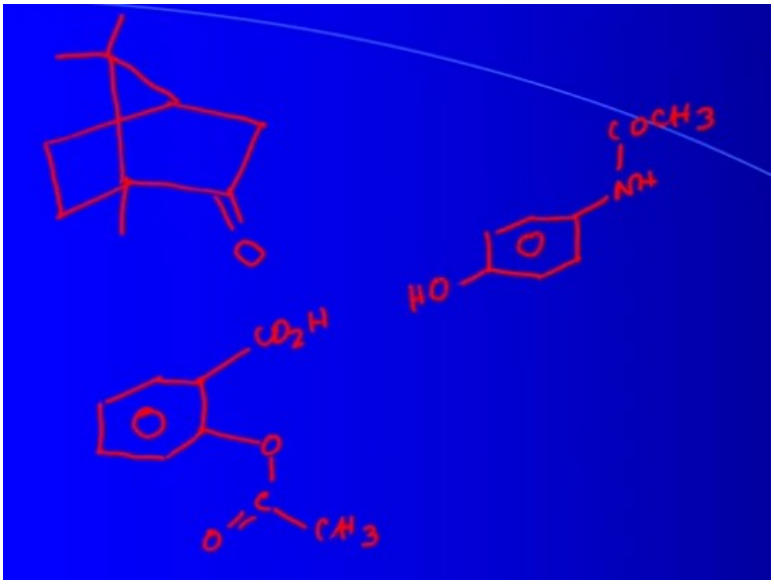

The first molecule is a bridged molecule that you may see here, the second molecule that I want to draw is the following. And the third molecule is this one so try to write down the name of these 3 molecules. Thank you.