Symmetry, Stereochemistry and Applications
Dr. Angshuman Roy Choudury
Department of Chemical Sciences
Indian Institute of Science Education and Research, Mohali

Module No # 01
Lecture No # 02
Nomenclature of Various Organic Molecules

Welcome back to this course on symmetry stereochemistry and applications. So let us start the lecture today from the point where we stopped in the last class. We were trying to understand the nomenclature of various organic molecules. So in that I had given you one small problem to identify the name of a given molecule.

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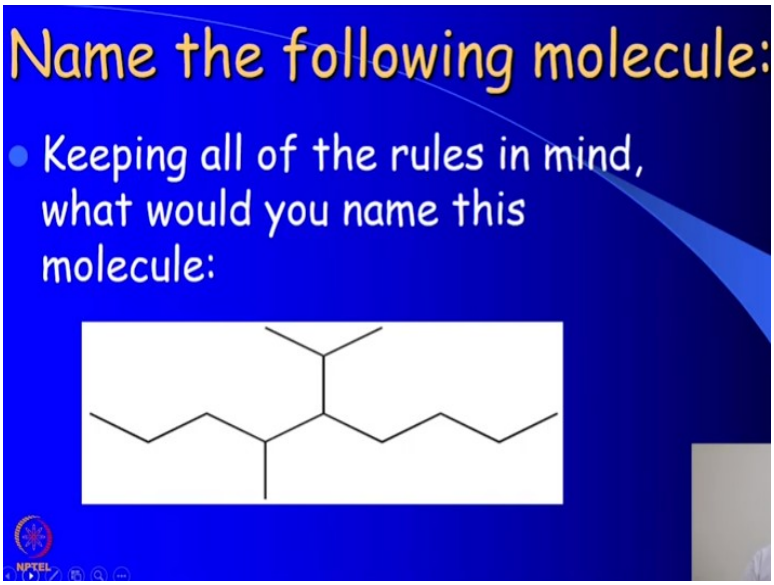

So what I gave is this particular molecule, I said keeping the rules that we have already discussed we try to identify the name of this molecule. So let us see what the solution is.

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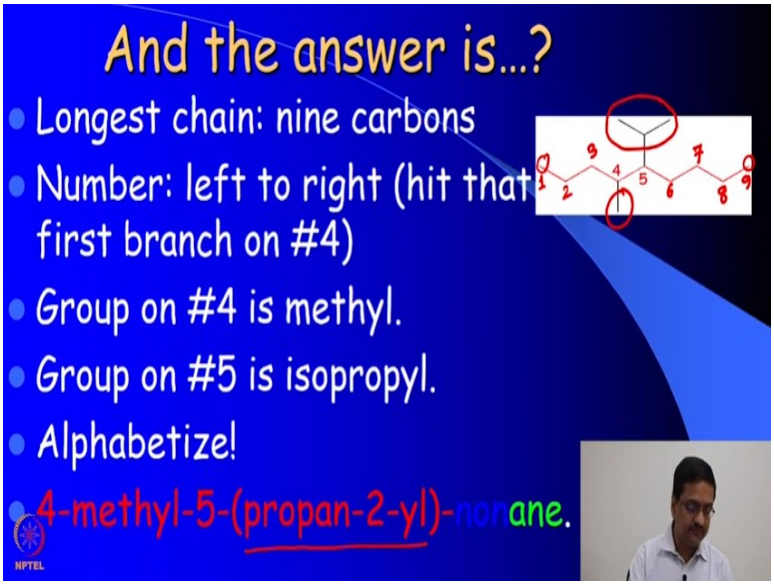

So what we should try is, we should first try to identify the longest chain in this molecule. So when you try to see that what we find is, if we are trying to number it from the either side, either from the left corner or from the right corner we get the same thing like 1, 2, 3, 4, 5, 6, 7, 8 and 9. So it means that the molecule is a 9 carbon hydrocarbon and it is called the nonane. Now we need to find out the substitutions that are present so what we see very easily that there are 2 groups that are attached one is at number 4, a methyl group.

And the other group at number 5 which is slightly larger group which is a propan-2-yl or isopropyl group. So when you try to name it we should start from the lowest numbering where the 4 is methyl and 5 is isopropyl are more appropriately propan-2-yl. So the name of that molecule will be 4-methyl-5-(propan-2-yl)-nonane. Hope you are able to follow this scheme of nomenclature.

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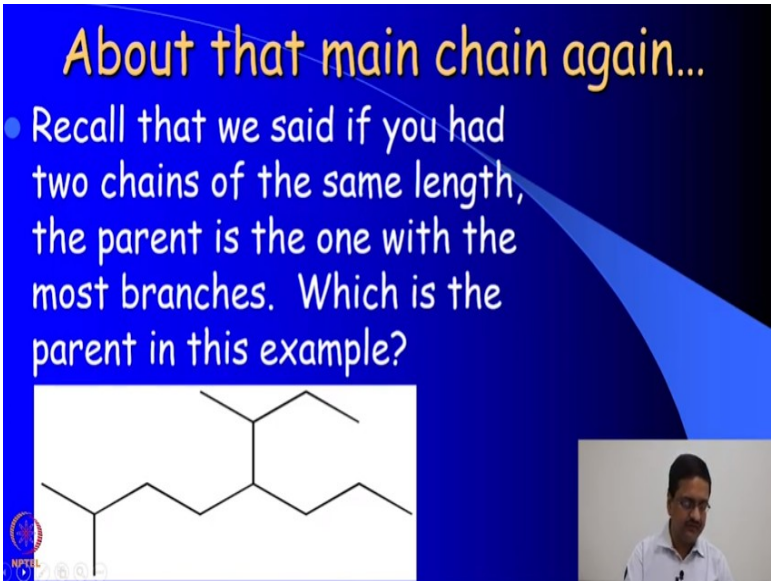

So when we are trying to identify the name of the molecule what we need to worry about is first to find out what is the main chain of this particular molecule? What is the length of the main chain and how to number that?

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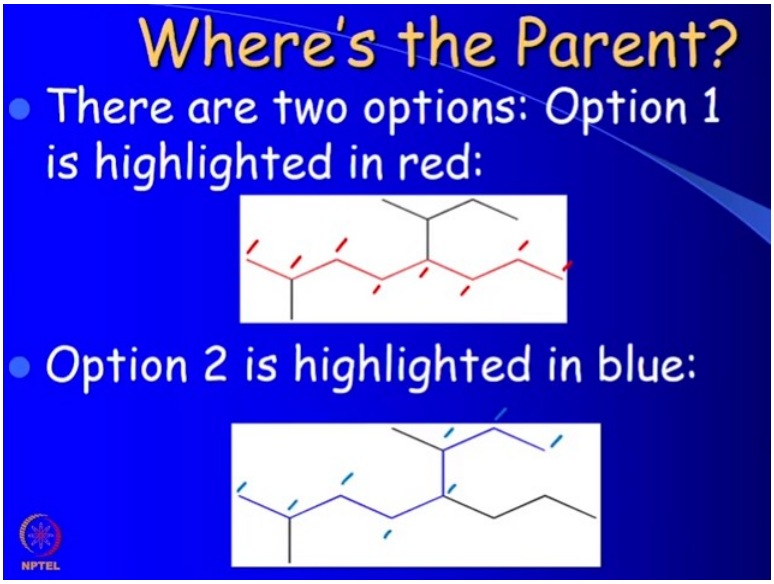

So in this particular molecular molecule that I am showing here there are 2 possibilities of considering the main chain. In the first figure on the top what you can see is I have marked with red the long chain which has 1, 2, 3, 4, 5, 6, 7, 8 carbons. In the lower figure that I have shown I have marked the longest chain using blue. So you have 1, 2, 3, 4, 5, 6, 7, 8 so now what we have is in both the cases we have 8 carbon atoms. Now the question is which one to take which one is my longest chain how do I number it?

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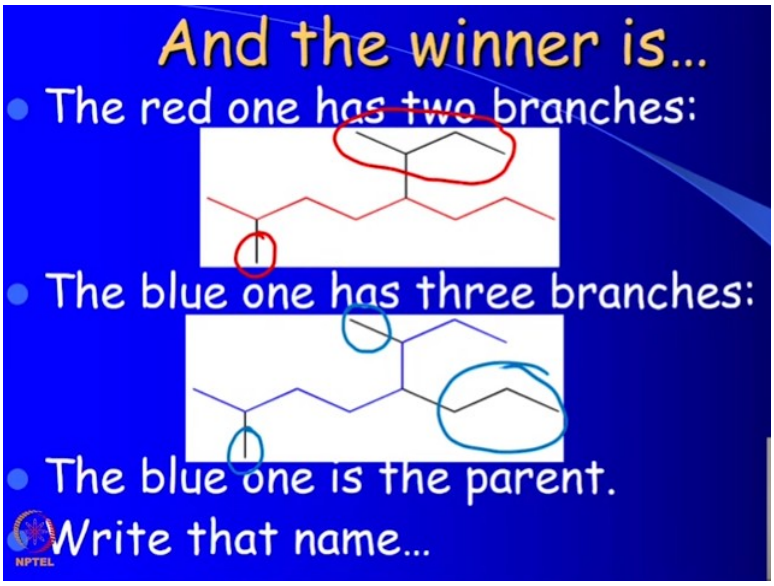

So we need to add now a new rule when you are trying to number a long chain in this manner one has to look at that how many branches are there associated with a given long chain. So what we see in this particular case when we are looking at the top drawing where you have the longest chain of 8 atoms drawn in red you have 2 substitutions 1 and 2. And in the lower case if we look at the blue chain we have 3 substitutions.

So when you have 3 substitutions in the blue parent chain that we must identify the longest chain as the blue chain and then try to write the name of that molecule in that fashion.

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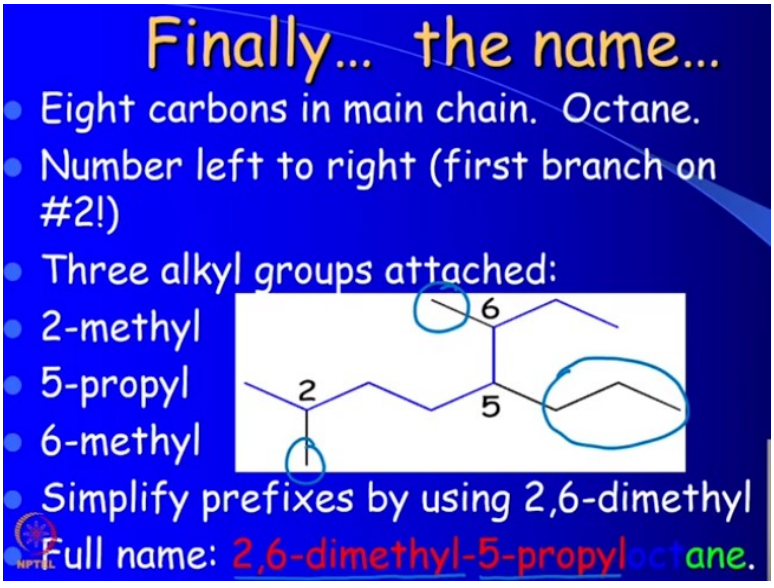

So when we try to write the name we should write the atom numbers starting from left to the right and then try to write down the name of the molecule using the appropriate prefixes; those are the substitutions that you have on the main chain. So now what we have is at 2 position and 6 position we have to 2 methyl groups so that we write as 2,6-di-methyl at 5 position we have an isopropyl group sorry we have a propyl group so we write it as 5 propyl and the main chain is octane. So we write it as octane so the full name will be 2,6-di-methyl-5-propyloctane.

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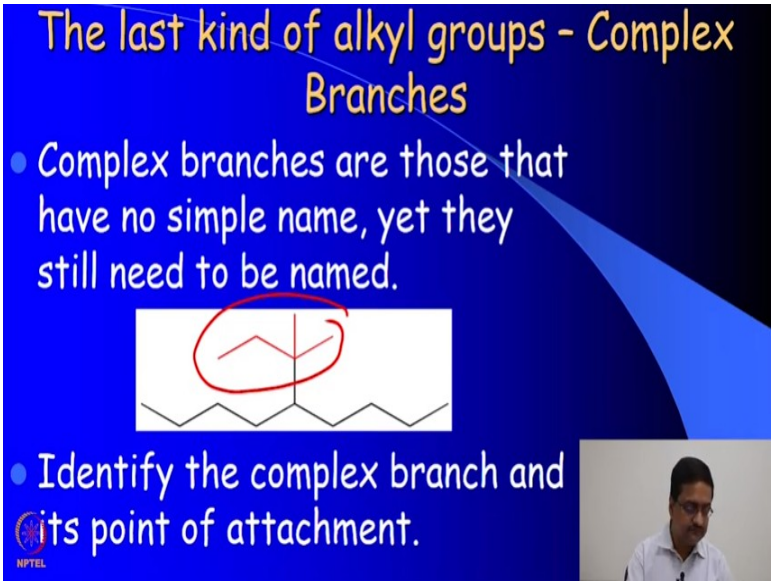

Now we need to worry about a new type of branching which we have not addressed before. The last kind of alkyl group which has a complex branch. Here what we mean by complex branch is a complex branch are those that have no simple name yet they still need to be named in a molecule. So in this particular case if you look at the branch that is drawn in red, this part is different from what we have seen before. So we need to name this complex branch using a set of rules.

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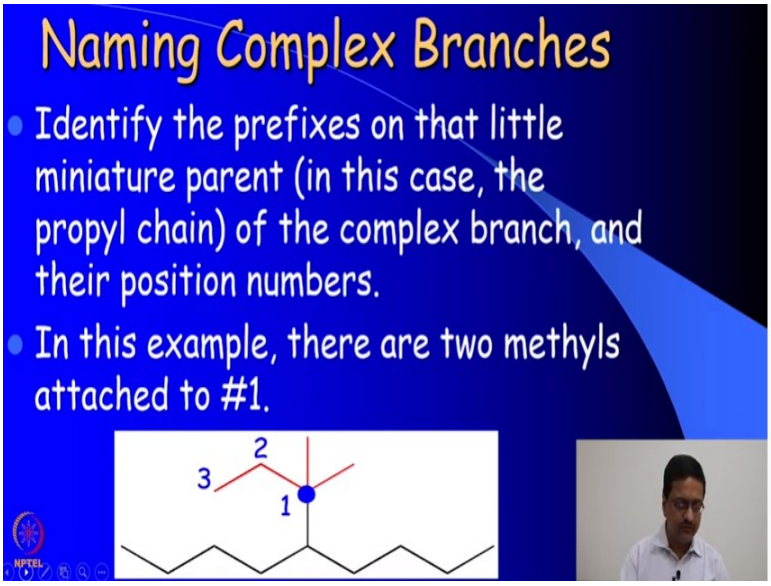

So when we try to do that what we need is to find the point of attachment inside the complex branch itself. So here what you can see in the red branch you have a blue dot that blue dot identifies the point through which this particular branch is attached to the main chain. So now considering that blue point as the point of attachment we need to identify the number of carbon atoms present in the longest chain in the complex branch.

So starting from the blue dot we can write the longest chain as 1, 2 and 3 remember that we should write that as 1 not the chain that comes like this as the longest chain. So what we do is then we try to write the name of complex branch so when you have 1, 2 and 3 identify the other prefixes that are present here. So in this particular example there are 2 methyl groups attached.

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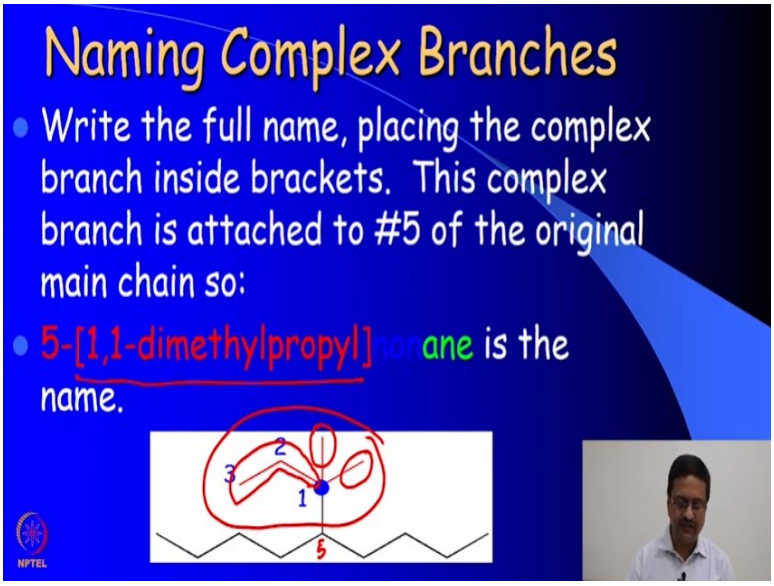

So when you have 2 methyl groups attached in this branch we should write it as, this group will have a name written here. At 1 position we have 2 methyl groups. So we write it as 1,1-dimethyl propyl is the name of that chain and this complex branch is attached at the 5 position of this molecule. So we write it as 5 in square bracket 1,1-dimethylpropyl nonane and this is the name of this particular molecule. So this is how one should name a complex branch in a given hydrocarbon or in a given molecule.

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Now let us move to the next part where we try to name the cyclic compounds. When we are naming the cyclic compounds we need to first determine the ring size of the parent and whether the parent is the ring or any other part of the molecule is the parent. If the ring has more number

of carbon atoms then any of the alkyl groups attached to it than the ring is called the parent ring. If not then the ring becomes a cycloalkyl group and these are prefix to the main chain so we should remember this.

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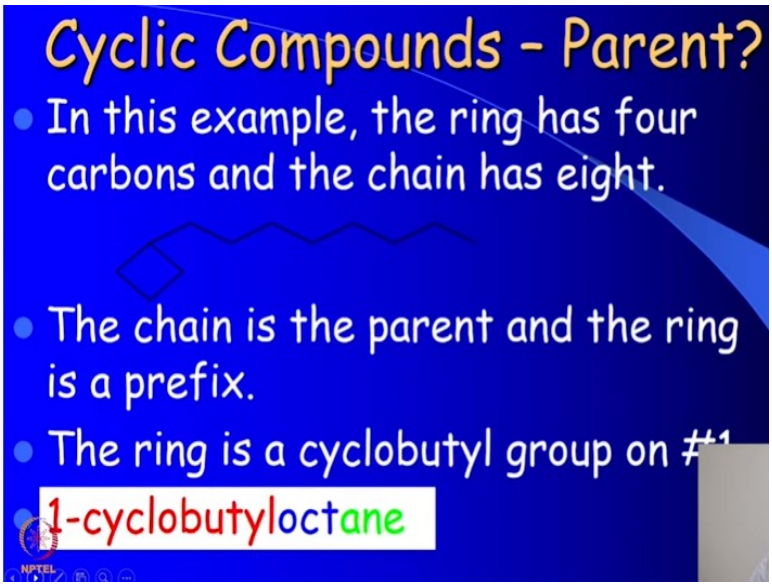

So when you have an example like this where you have a small cyclobutane attached to a large hydrocarbon, the chain is the parent. And the ring is the prefix so, in this particular case when you have a cyclobutyl ring attached to a chain we write it as 1-cyclobutyloctane. Because the parent, the chain as more number of carbon atoms compared to the number of carbon atoms present in the ring.

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Now we continue in this cyclic compounds now in this case you see here the situation is opposite. You have the molecule where the ring has 5 carbon atoms and the side chain has 3 carbon atoms. So 5 carbon atom ring is the parent and the side chain is the prefix so like that when we try to name the molecule we write it as propylcyclopentane and this is the name of this particular molecule.

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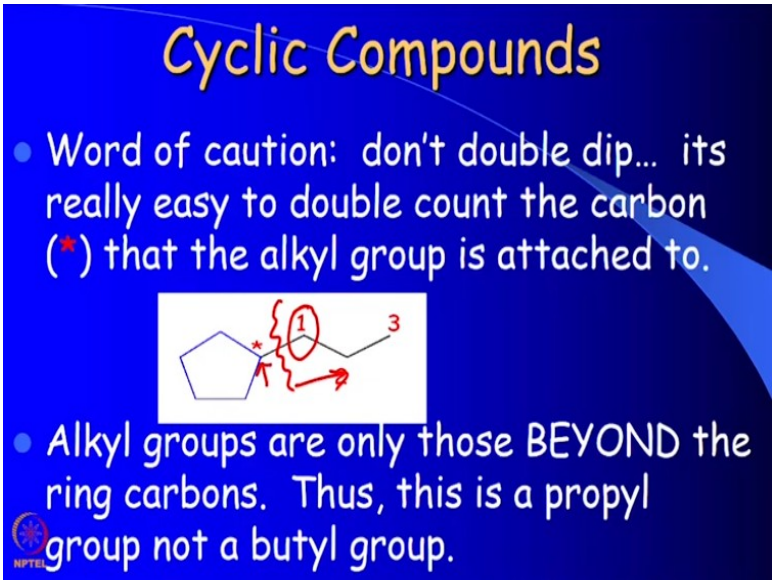

What we need to remember here is that we should not double count the atoms that are connected to the side chain. The side chain is starting at this point of attachment so from here this side chain is attached, so the side chain length has to be considered from this side to the other end. We should not count that atom at which this side chain is connected along with the number of carbons in the side chain we should not count that atom twice.

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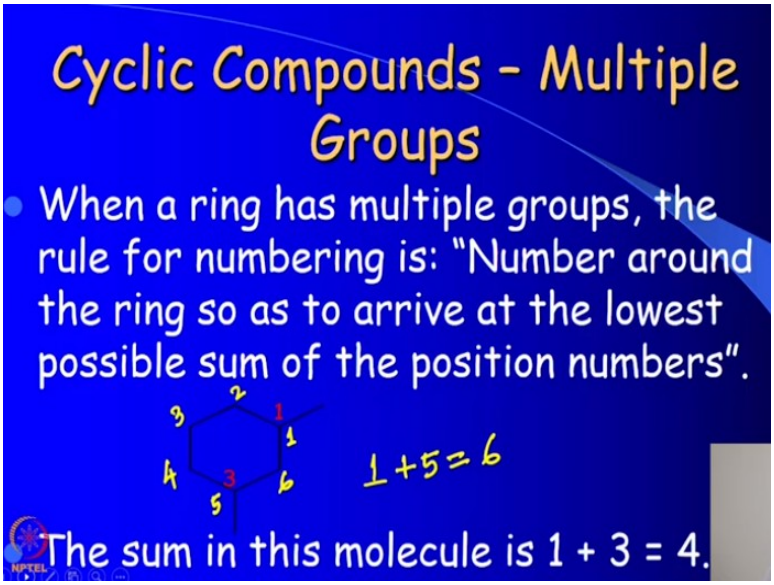

Now we need to see what we happens when we have multiple groups present in one particular cyclic compound. What we need to do is we then need to give numbering and those numbers should be such that this sum of the numbers coming on the substitution should be minimum. So for example in this particular case the way is written here is one way of writing it I can write it as 1, 2, 3, 4, 5 and 6.

So in this particular way when you write the number in yellow what we see the sum of those 2 numbers becomes 1 + 5 = 6. This number 6 is larger than 4 so the way that was numbered in red is the right way of numbering.

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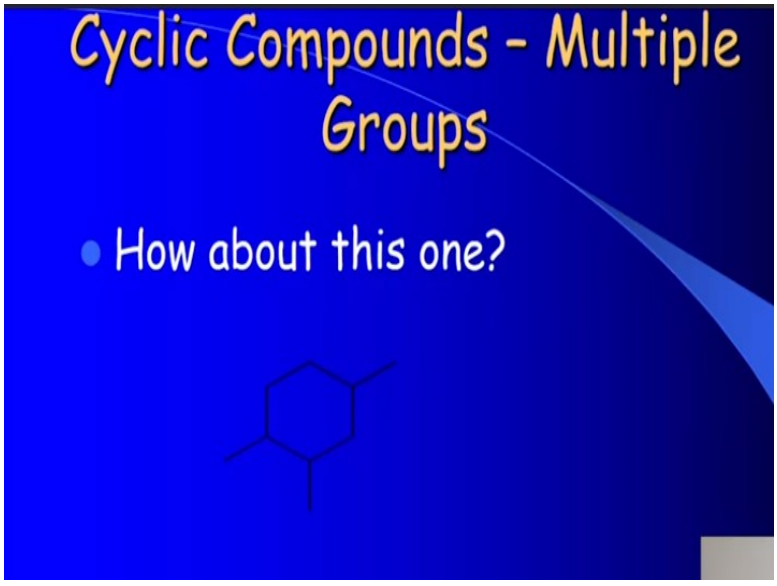

So 1 + 3 so when we write the name of the molecule it we should write it as 1,3-dimethylcyclohexane. How about this particular compound how should we name this molecule?

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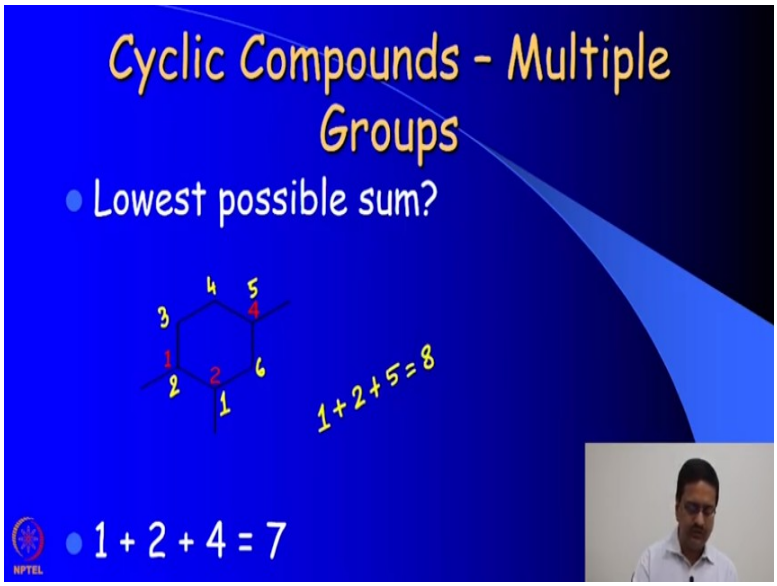

When we have 3 different functional groups 3 different prefixes we again write the numbers in such a way that the sum of those 3 numbers is the lowest. So here we write it in the anti-clock wise direction starting at 1 to 2 to 4 and the sum is 1+2+4. If we has started from the point 2 and written it in the other direction then what you would have got is different. If you had started from here as 1, 2, 3, 4, 5 and 6 in that case it would have been 1 + 2 + 5 = 8 which is larger than 7.

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So as a result the name should have been different. Now we have another possibility, We have 2 different groups attached to a cyclic compound, so when we have 2 different groups attached to a cyclic compound what we need is we need to priorities them using their first alphabet of the name. So we should alphabetize each of them and we should try to write the name of that compound. So look at the molecule here it has, on right hand side a 2 carbon atoms and the left hand side it has 3 carbon atoms the groups are different one is isopropyl and the other one is ethyl.

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So when we try to write the name of that compound we have to number it in such a way that we get the lowest sum. Now in any direction if you write methyl as 1 and isopropyl as 3 it is 3+1, 4. If you write isopropyl as 1 and ethyl as 3 then it is 1 + 3; so that both ways it is the same. So while trying to name it we should again alphabetize to give the number and we assign number 1 to the ethyl group.

And then number 3 to the propan 2-yl group or the isopropyl group and we write it the name as 1-ethyl-3-(propan-2-yl)cyclopentane. Hope you are able to follow this type of nomenclature.

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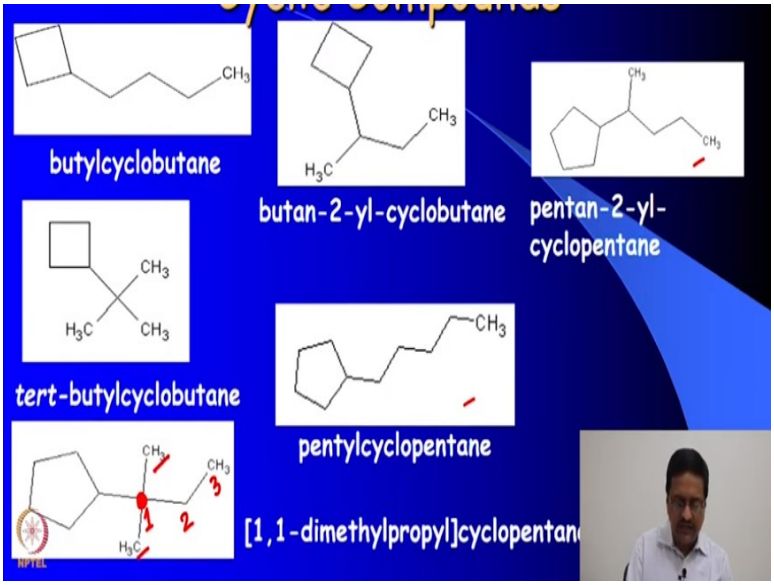

So we continue the understanding on cyclic compounds. See here I am giving you a few examples. What is happening here can you see the number of carbons, that are present in the ring and the number of carbon atoms present outside the ring is one and the same. And the way we have named this molecule is unique. So in the case of the first molecule where we have a cyclobutyl ring and we have a butyl chain attached to it we have named it as butylcyclobutane that means the parent is cyclobutane and butyl is a substitution.

Similarly second one is written as butan-2-yl-cyclobutane the third as tert-butylcyclobutane, this one as pentylcyclobutane sorry this one as pentylcyclopentane. And the last one as pentan-2–yl-cyclopentane so what is the logic behind this type of writing? The logic behind this type of writing is that the group cyclobutane is unsaturated hydrocarbon. So the unsaturation creates priority over a saturated chain.

So the unsaturated chain gets the name of the parent and the side chain is written as a prefix and that is why when the outside and inside that is ring and the chain has the same number of carbon atoms, the name is given with the cycloalkyl as the parent and the other part as the prefix. You have one more such example which has a complex branch that you can see and again the complex branch is named as we have understood in this class a few slides before.

So here we have the side branch which is connected at this point so here we write it as 1, 2, 3 and then we have 2 methyl groups and those 2 methyl groups are named as 1,1-dimethylpropyl cyclopentane.

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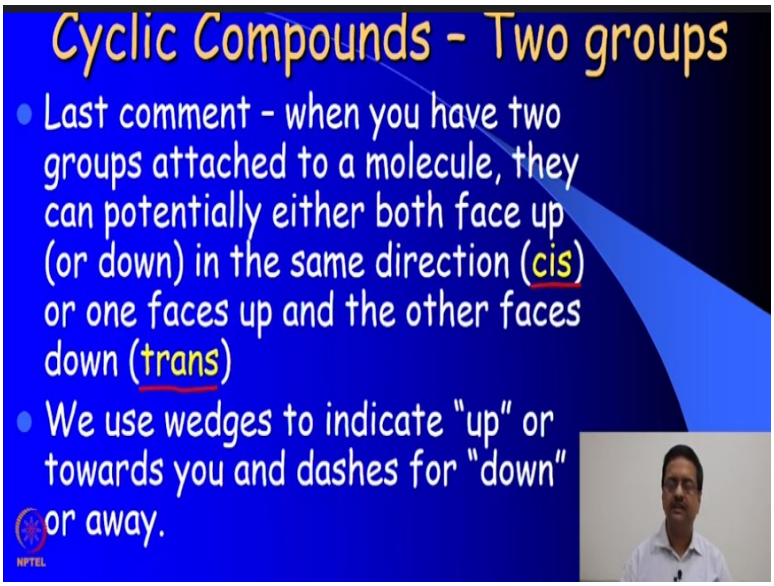

Now in a cyclic compound as you know it is a ring molecule and when you have a molecule which is a ring it is possible that the substitutions that are present on those 2 carbon atoms can both be up can 1 be up and other one be, down. So when you have such conditions that 2 alkyl chains or 2 groups attached to a cyclic compound are spatially oriented in different ways either both are upwards pointed upwards or one pointed upwards and other one pointed downwards.

We should identify those 2 molecules as 2 different molecules and when we try to write that we try to understand them in the form of cis and trans. When the 2 groups are pointed in same direction it is called the cis. When the 2 groups are pointed opposite side that compound is called the trans.

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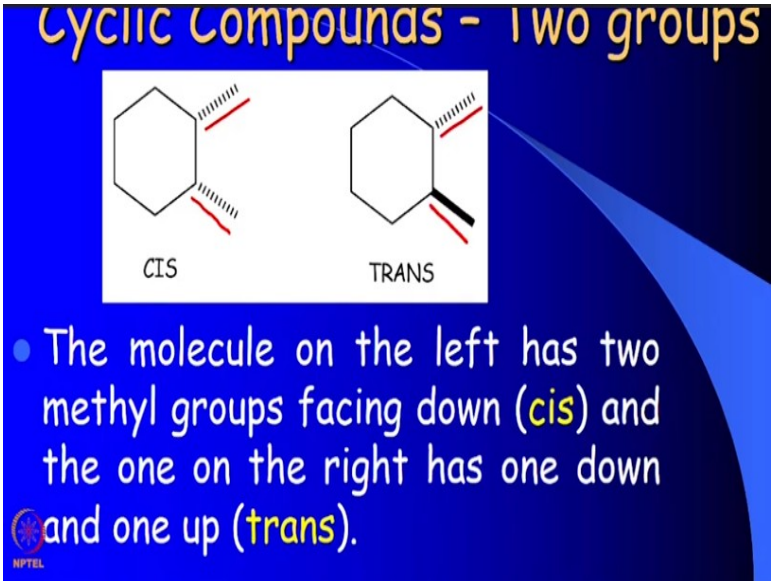

So when we try to draw that in a 2 dimensional projection using wedge and dash formula when you write this type of wedge instead of dash formula and that identifies that this is the trans molecule.

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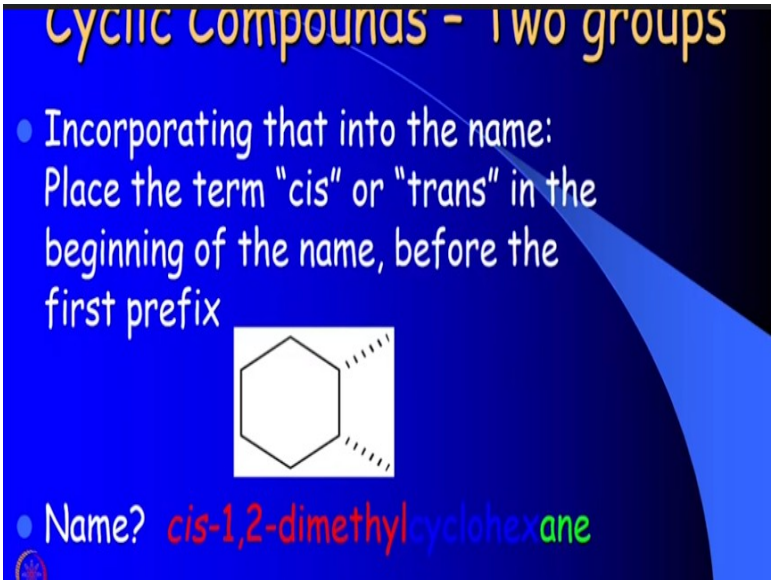

So when you have such a molecule you try to write down the name as 1,2-dimethyl cyclohexane. And when we see that the 2 groups are on the same side we add a small term as cis the prefix to a prefix which is cis- 1,2-dimethylcyclohexane.

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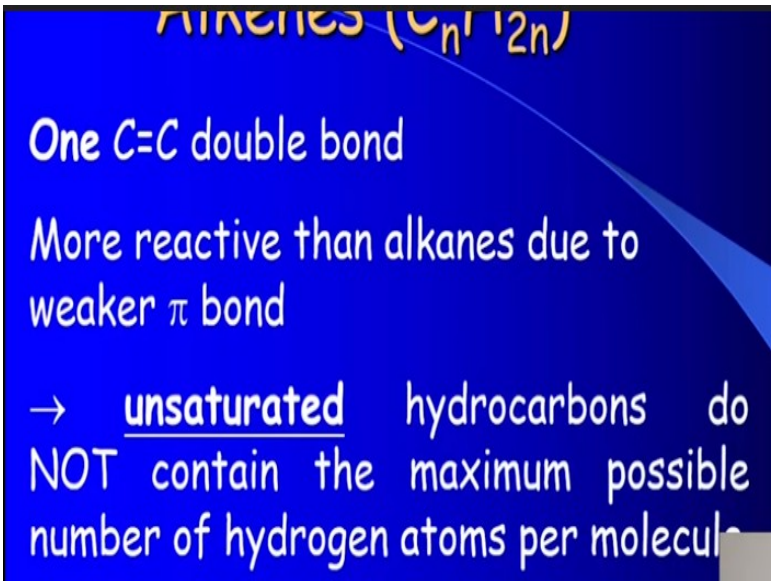

Now let us move to the next set of molecule which are the alkenes where you know that there is unsaturation so there will be a C=C double bond. And they are reactive than alkanes due to weaker pi bond and they are called unsaturated hydrocarbons and do not contain the maximum number of hydrogen's that are possible for a given number of carbon atoms in a hydrocarbon.

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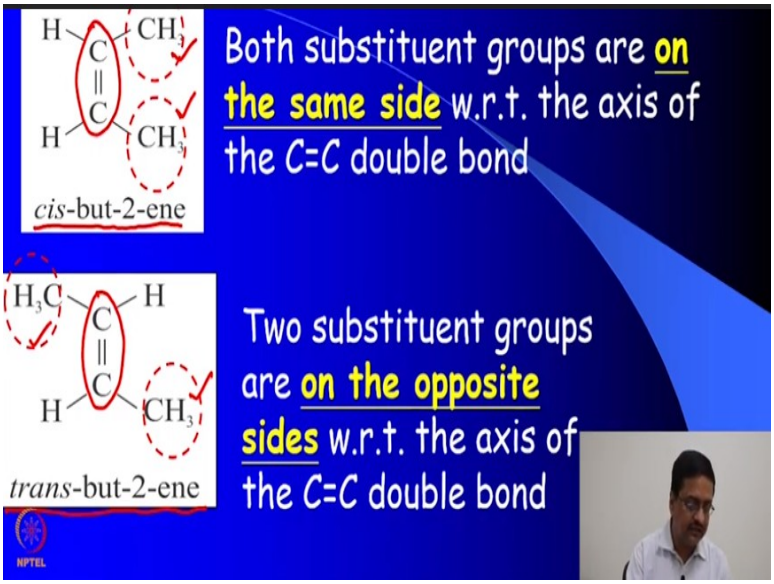

So in that also we can have a cis and trans different isomers and here in this particular example where you can see on the top you have a C=C double bond in the middle. And that C=C double bond has 2 methyl groups attached and both of them are on the same side. So we call that as cis but-2-ene and the other molecule that you have in the lower bottom end of the slide you have a double bond and the 2 methyl groups are across the double bond on 2 sides.

So this molecule is called as the trans-2-butene these things are actually taught in your 10 + 2 but I would like to cover this as a follow up because you may have forgotten many of the things that were learnt in your 10 + 2.

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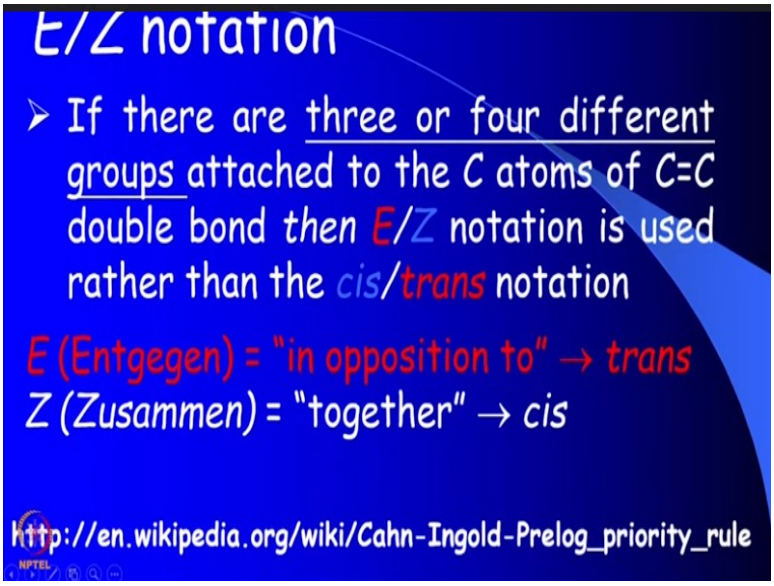

So when we have a C=C double bond and if there are 3 or 4 different groups attached to a double bond then we try to write them as E or Z instead of cis and trans. So E in German means Entgegen and that means it is in opposition to which is equivalent to trans. And Z in German is Zusammen which means together which is equivalent to a cis. So this nomenclature can be found in this particular link where you can get all possible rules of this cip nomenclature of organic compounds.

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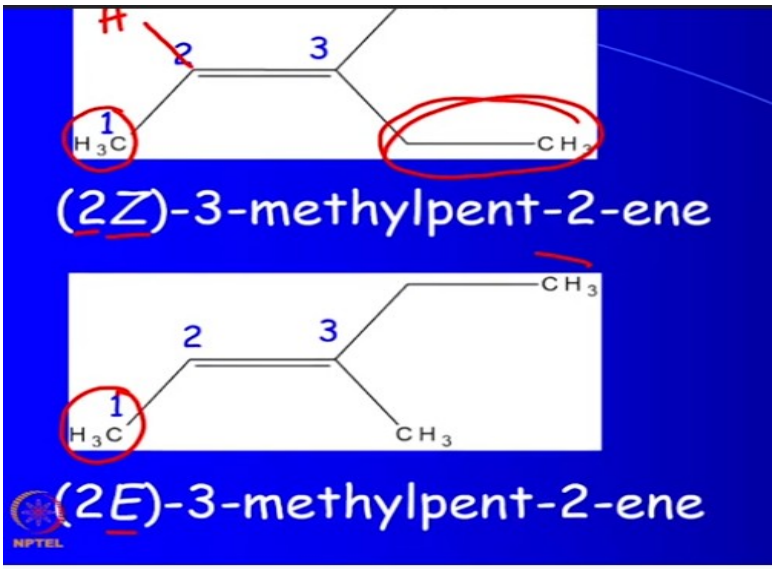

So here what we can see in the molecule, this 2 molecules have same formula but the groups that are attached are in different way. So, both of them have 5 carbon atoms in the longest chain and the groups that are attached are attached in different directions. So what we see here is that we try to prioritize the position of the atoms on either side of the double bond. So in the upper molecule the hydrogen atom is attached here.

So on the upper molecule the priority on the carbon number 2 is for the methyl group and on third carbon the priority is on the ethyl group. So here the 2 most prior groups are on the same side and it is equivalent to cis that means in the E/Z nomenclature it is Z and this 2 that appears is the position of the double bond from where it starts. So we write it as (2Z)-3-methylpent-2-ene. In the lower case the first higher priority methyl group is down and on the other side the higher priority methyl group is up.

So these 2 are in opposition to and that means it is entgegen or E so we write it as (2E)-3-methyl-cyclopent-2-ene. So this is how these 2 molecules should be named and they are different as you can easily see.

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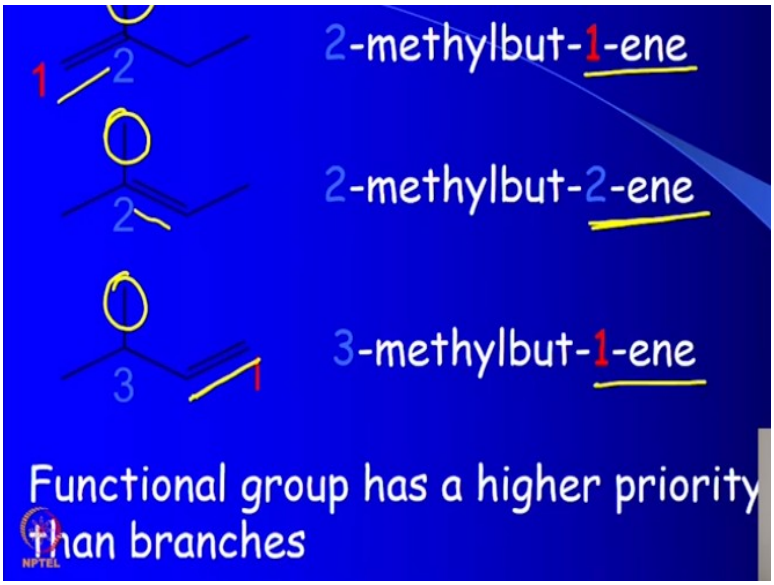

So here are some more examples of a double bonded compound, you can see the names of these molecules. The first one is named in such a way that you have the double between the 1 and 2. Second one the double bond between 2 and 3 and in the third case the double bond is again between 1 and 2 but on the other side because the position of the double bond when it changes it decides the way it should be numbered.

So functional group has higher priority than branches so in this particular case when you have the first molecule it is 1-ene. In case of the second molecule it is 2-ene and in case of third molecule it is once again 1-ene. So the ene gets higher priority over the functional group and then sorry ene gets priority over the branches. And now in case of first case when you have written it numbering from the left hand side 1 and 2, the alkyl chain is coming at the 2 position so it is 2-methylbut-1-ene.

In second case we write it as again at a 2 position you have the substitution so that is again 2-methylbut-2-ene. But in the third case the substitution that comes is at 3 position so we write it as 3-methylbut-1-ene. So with this we will end our lecture here and we will continue from this point in the next class. Thank you.