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 # 01
Introduction to Stereochemistry

Welcome to the course entitled symmetry stereochemistry and applications I am Dr. Angshuman Roy Choudhury, the instructor of the course and with me there will be tutors Dr. Sagarika dev from MCM DAV college for women and my PhD student Ms. Labhini Singla. So, they will be available through email for any questions and discussions. And I am also available at the email that is given at the bottom of this page.

So before I start I would like to introduce myself I have done my PhD from Indian Institute of science Bangalore and I completed my degree in 2004 and afterwards in 2005 the degree was awarded. I worked in the University of Liverpool for about 3 years from 2004 October to 2007 September, after that I joined Birla institute of technology and science (BITS) pilani and worked there an assistant professor in chemistry for 2 years.

And then I moved to Indian Institute of Science education and research at Mohali in the month of December 2009. And since then I am an assistant professor at this institute.

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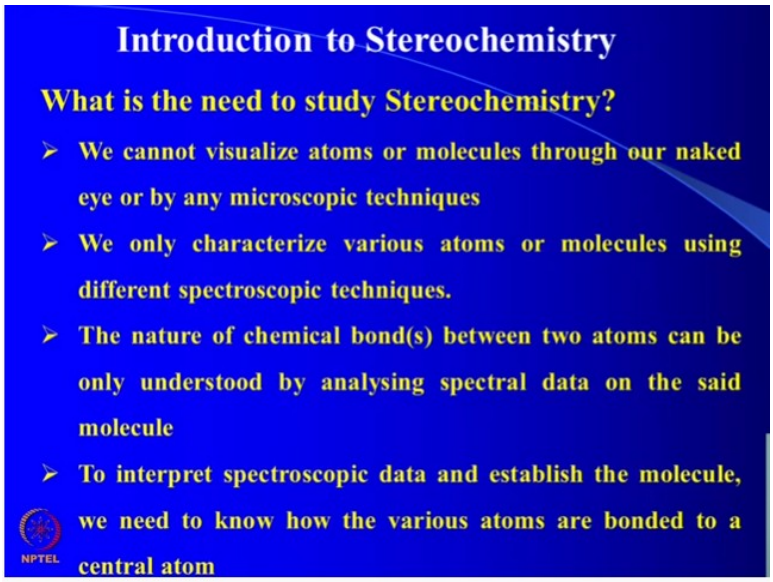

So in this particular course we are going to discuss about the stereochemistry, applications of symmetry in stereochemistry and a large number of chemical reactions which are really important in synthetic chemistry. So when we try to learn the word stereochemistry first thing that comes to your mind may be what is the need to stereochemistry why do we want to study something called stereochemistry?

As you all know that we cannot visualize any atom or any molecule using any microscopic techniques and of course not even through our naked eye. We only characterize various organic molecules or atoms using different spectroscopic techniques. And the nature of chemical bonds between 2 atoms can be only understood by analyzing spectroscopic data on that particular molecule.

So to interpret spectroscopic data and to establish the molecule we need to know how the various atoms are bonded to a central atom. So that means we need to know the stereochemistry that is the 3 dimensional arrangements of atoms around the central atom to identify the molecule and its geometry.

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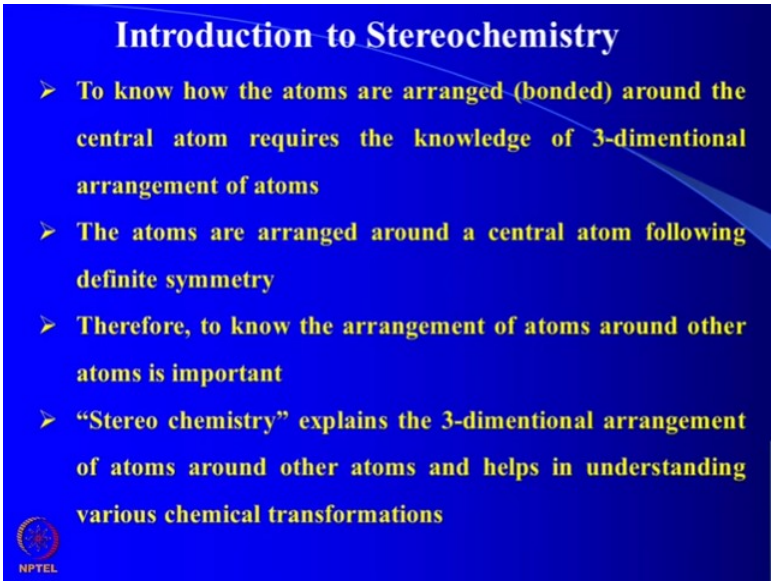

So to know the atoms that are arranged or bonded around the central atom that requires, knowledge of 3 dimensional property of that particular atom. The atoms that are arranged around the central atom they follow a definite symmetry. Therefore to know the arrangement of atoms around the other atom is very important. So we need to know the symmetry that is present in a

molecule and then the symmetry that gives rise to a particular molecule with different atoms arranged around a central atom.

So the word stereochemistry explains the 3 dimensional arrangements of atoms around the other atoms and helps in understanding various chemical transformations. So as a chemist when we try to identify the symmetry elements present in a molecule we try to utilize our knowledge of symmetry and identify those molecules in different groups. At the very onset we need to know how to name a molecule.

Because when we do not know how to name a molecule we may start naming the same molecule in different ways and create confusions in future. So therefore we need to have a common platform for naming organic molecules. As a matter of fact the naming should be done for all organic inorganic organometallic molecules in a uniform manner. So that the name is unique and everybody understands one particular molecule with one name.

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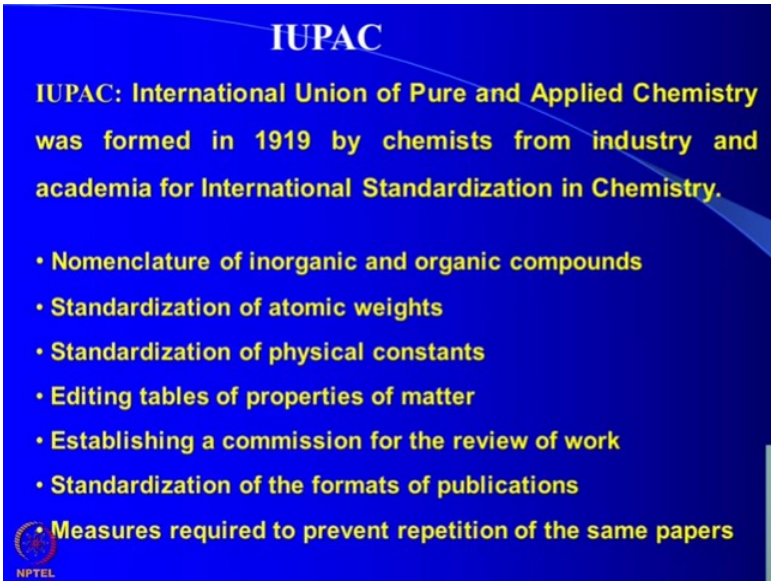

So as many of you have already come across the term IUPAC which is the short form of International Union of Pure and Applied Chemistry, which was founded in 1919 about 100 years ago by chemist from industry and academics for international standardization in chemistry. So initially the main goal of this union was to give a suitable nomenclature of inorganic and organic compounds, standardize the atomic weights of various different atoms and their isotopes.

Standardization of physical constants, editing tables of properties of matter so that one person can go to one particular table and get information about many physical properties of different elements. Then their goal was to establish a commission for the review of the work from time to time basis and standardization of the formats for publication and measures required to prevent repetition of the same parameters the same papers that means there was a goal to keep one unique identification and the properties everything related to any atom that is invented or discovered to be listed.

And the molecular properties also to be listed in a concise database. So IUPAC gave a certain guidelines rules to identify different organic molecules. And we will start by learning how these organic molecules can be named.

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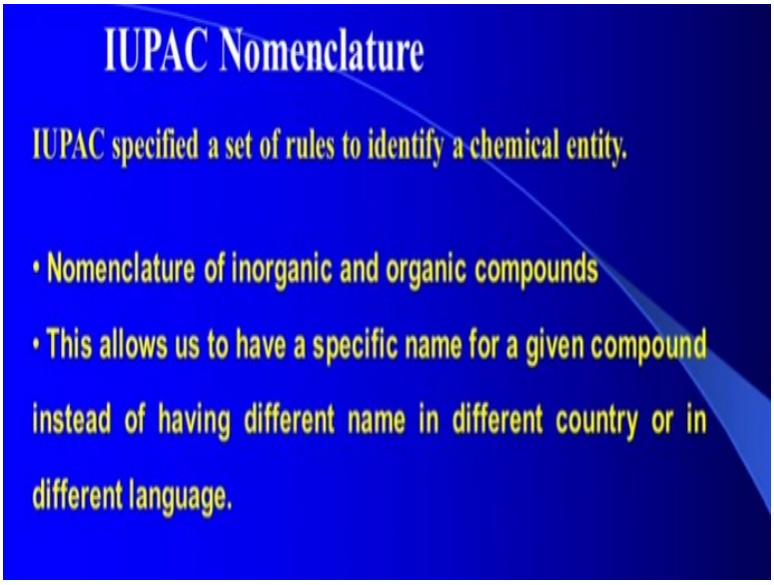

Some of you might have studied this IUPAC nomenclature in your previous years in your high school during 10 plus 2 studies. So we will initially go through the basic knowledge that you may have and then we will take you through some advanced parts of IUPAC nomenclature which will be certainly new to many of you. So IUPAC nomenclature; where IUPAC specify a set of rules to identify a chemical entity.

Nomenclature of inorganic and organic compounds were given. This allows us to have a specific name for a given compound instead of having different names in different country or different language.

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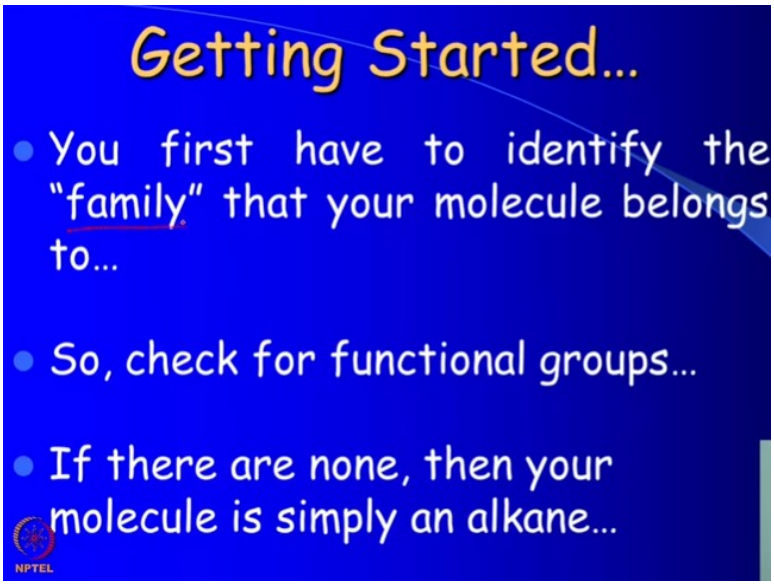

So let us get started because you see some of us as already studied some of these rules in our previous class but for everybody who may not have done it I would like to take you from the very beginning. So when you start trying to write a name of a compound you first have to identify the family that your molecule belongs to. Just like for human being you try to identify a person with his or her surname. So that corresponds to the family name of that particular compound.

So the family name becomes important and we try to find out what family the compound belongs to, which essentially means we are trying to look at the functional groups present in the molecule we are trying to prioritize the importance of those functional groups and then identify the molecule and try to write the name. So the functional groups present in the molecule becomes important to identify the family of the molecule.

Of course there are different large numbers of molecules which are nothing but hydrocarbons there is no functional group present in that. So in that case the molecule is termed as alkane. Remembers when you have a double bond or a triple bond that is also considered as a functional group. So the molecules which do not have any functional group are simply alkanes.

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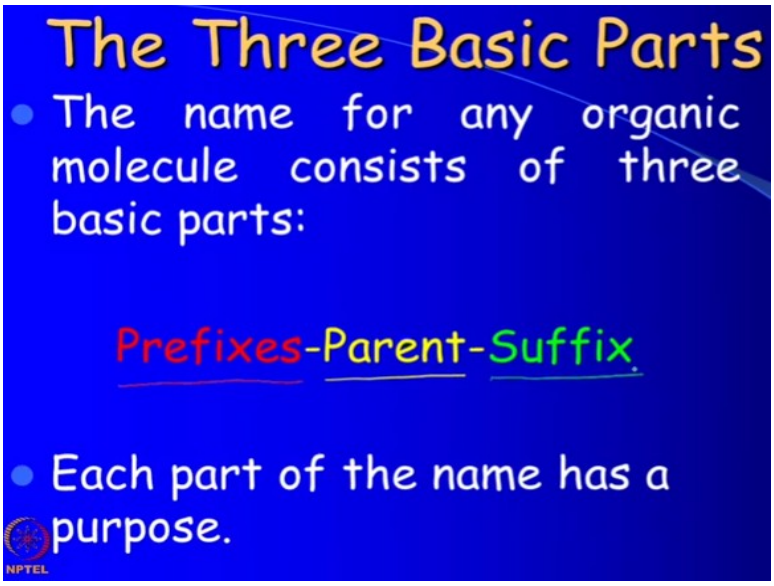

The name of a compound has 3 basic parts as you may see here the way the names are written, the name of the organic compound or molecule consists of 3 parts the first part is called the prefix or prefixes. The second part of the name is called parent and third part of the name comes from the family name that is the suffix. So the suffix identifies the family, the parent indicates the number of carbon atoms present in the molecule and prefix identifies what are the other substitutions that are present in your molecule?

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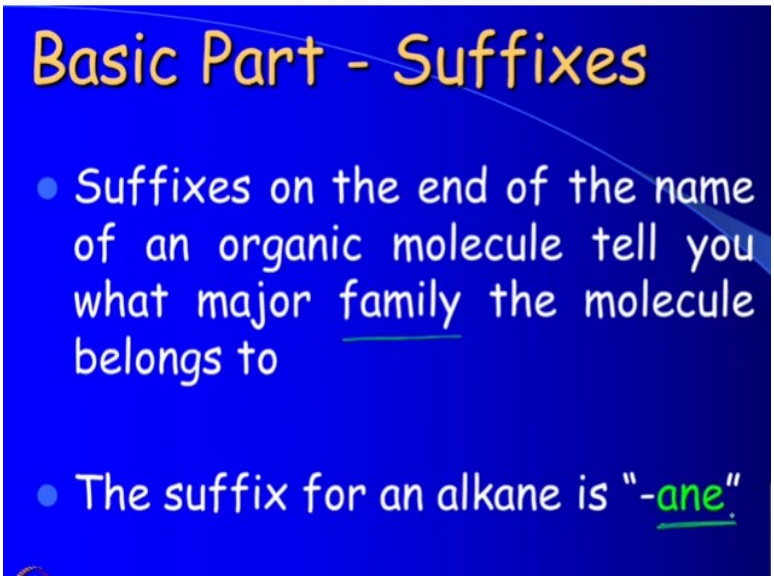

So first let us talk about the suffix. Suffix is on the end of the name of an organic molecule that will tell you what major family it belongs to. So whenever you have an alcohol the suffix will be ol. Whenever you have the aldehyde it will be al and so on which we will learn slowly one after

another when those compounds come. So in case of simple molecule like alkane the suffix for an alkane is ane and this should identify a molecule with the alkane family.

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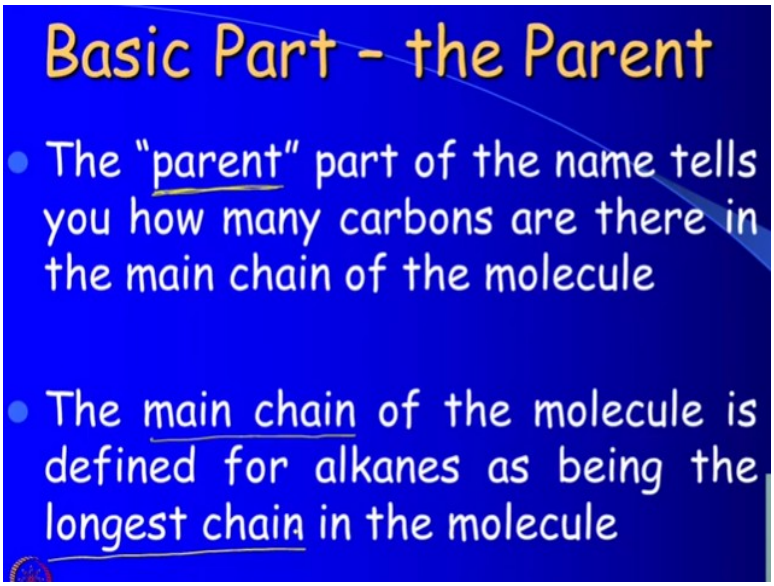

Then comes the basic part the parent so that parent is basically the part of the molecule which identifies how many carbons are present in that molecule. So it identifies the main chain of the molecule and is defined as the alkanes as being a longest chain of the molecule. So this term is very important so one has to find the longest chain to identify the parent of that particular molecule.

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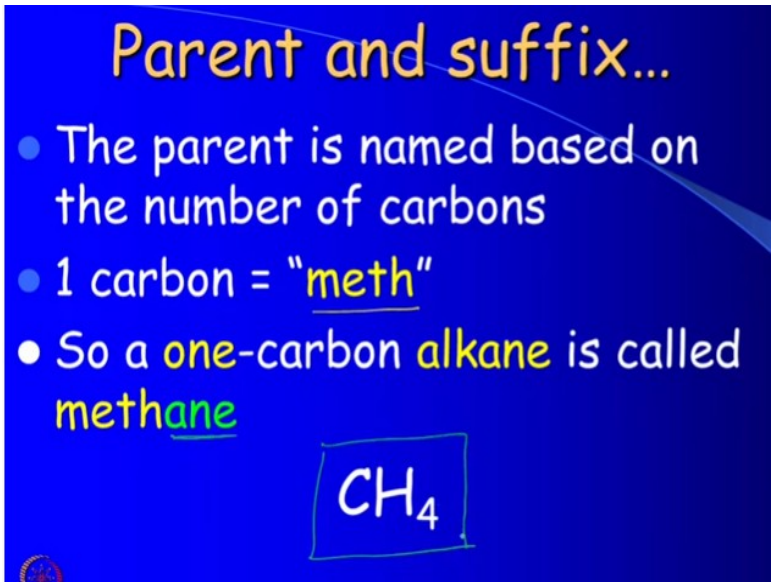

So now we talk about the parent and the suffixes first, so the first compound that one can think of is a single carbon compound; the methane. So the name has the word meth and the suffix that you write as ane that identifies the compound called methane which is a single carbon hydrocarbon, the smallest hydrocarbon that one can think of.

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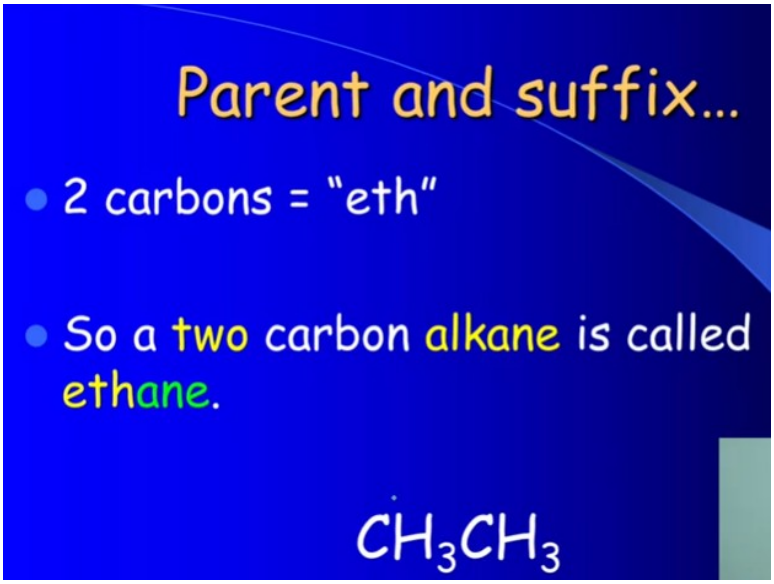

The second compound in the series is ethane which you all know.

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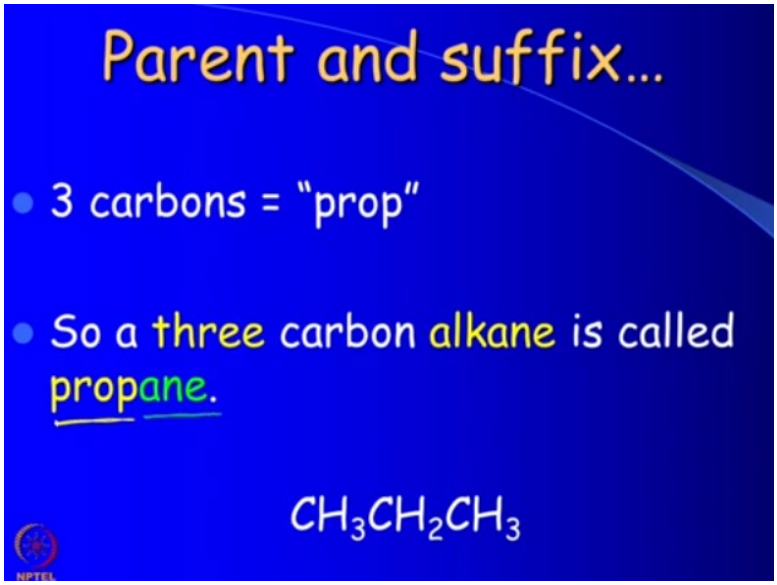

Similarly the third one with 3 carbon atoms is propane so as you can again see that you have as usual the ane which is identifying the family and prop that identifies the parent. So all these compounds the names have 2 parts parents and suffix and there is no prefix.

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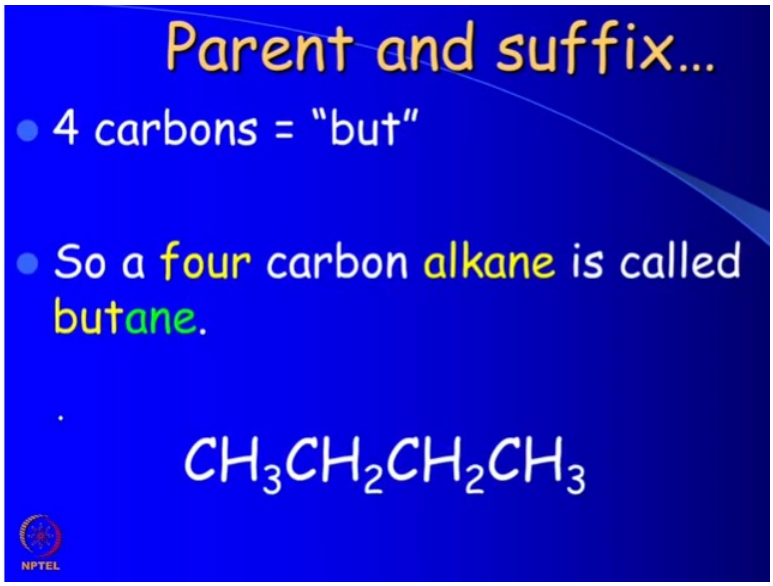

So like that when you talk about the next one is called butane.

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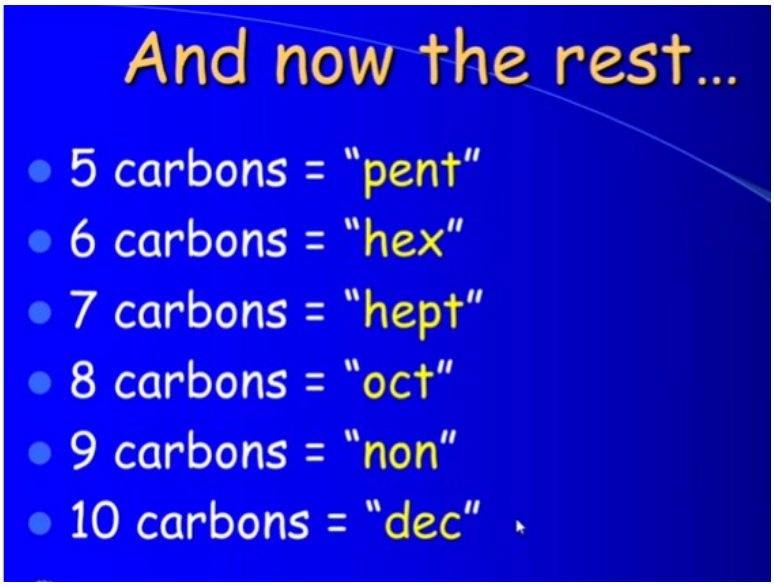

And so on for the rest you write it as pentane, hexane, heptane, octane, nonane and decane. These are the corresponding names of those compounds.

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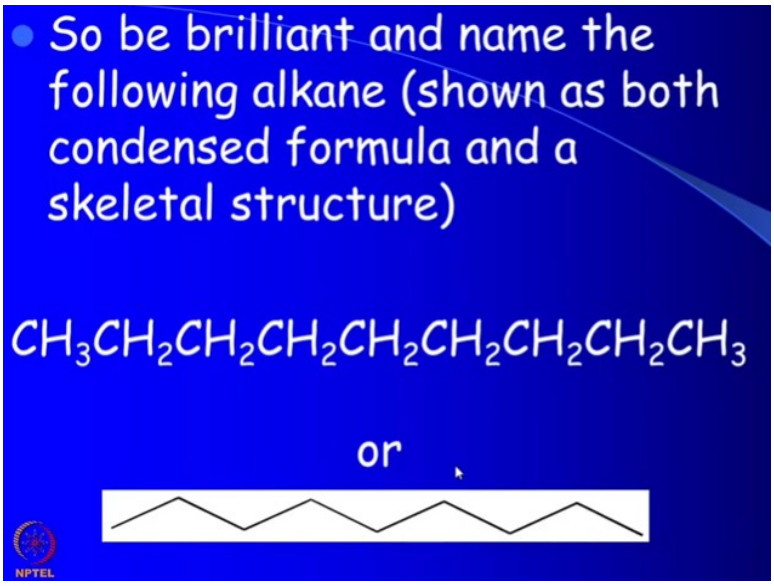

So great, so what should be the name of this compound let us try to count the number of carbon atoms present in this molecule 1, 2, 3, 4, 5, 6, 7, 8 and 9. So when you have 9 carbons it is called the nonane.

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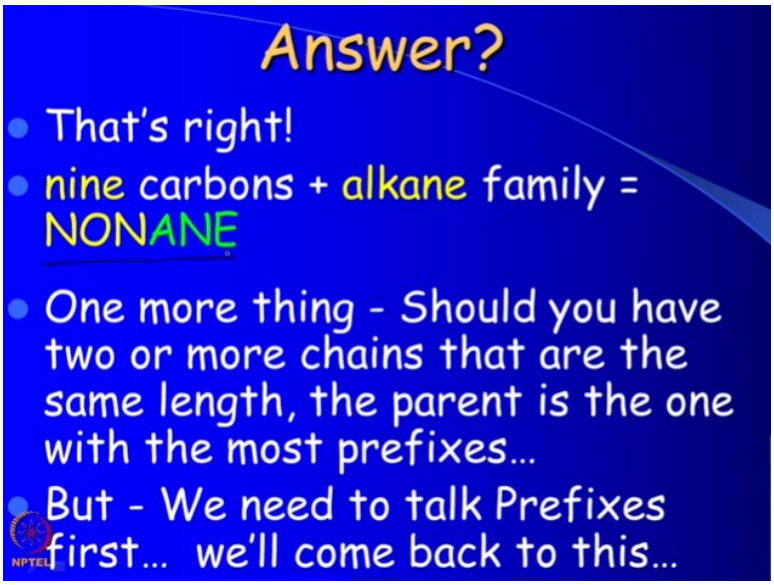

Nonane because 9 carbon atom compound, now we need to talk about the prefixes.

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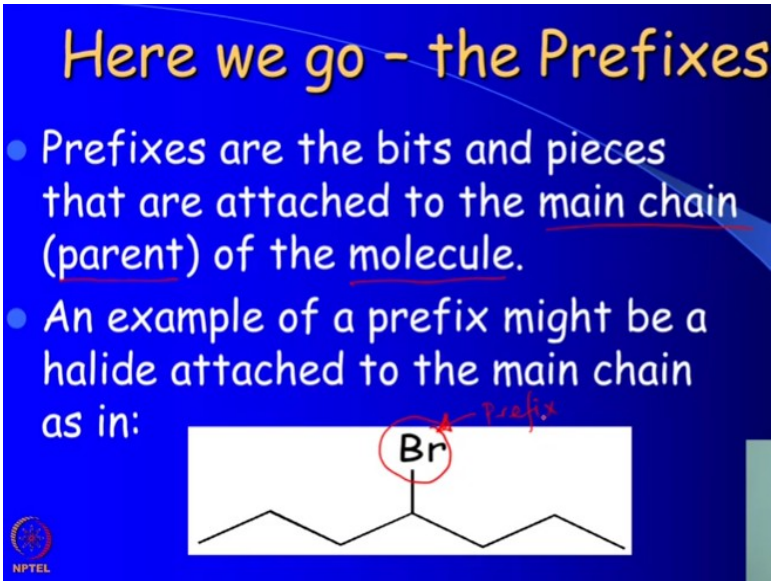

Suppose we have compound like this so what so we see here? We see that this particular compound has a hydrocarbon chain like that and a substitution in the middle. So prefixes are the bits and pieces that are attached to the main chain or the parent of the molecule. So this compounds name will appear as a prefix.

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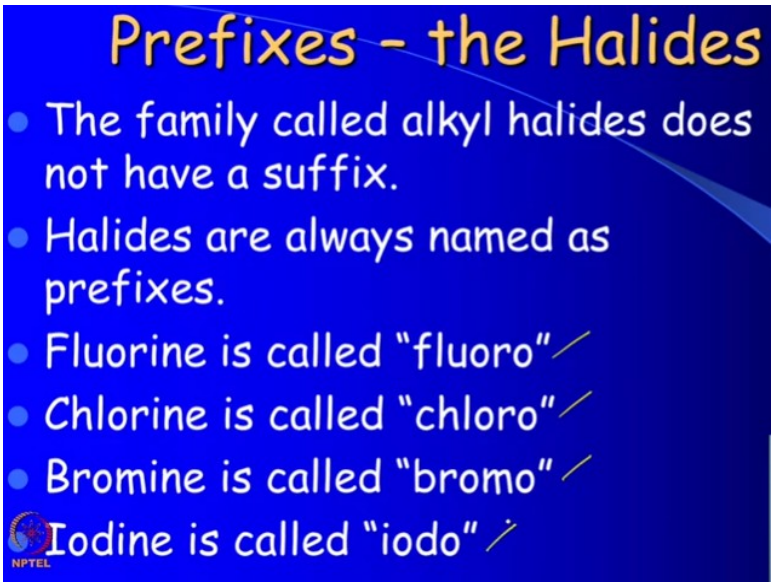

So when you have halogen as a prefix as you are seeing in this particular slide we may have fluorine, chlorine, bromine or iodine as a prefix. So we write those as fluoro, chloro, bromo or iodo as a name.

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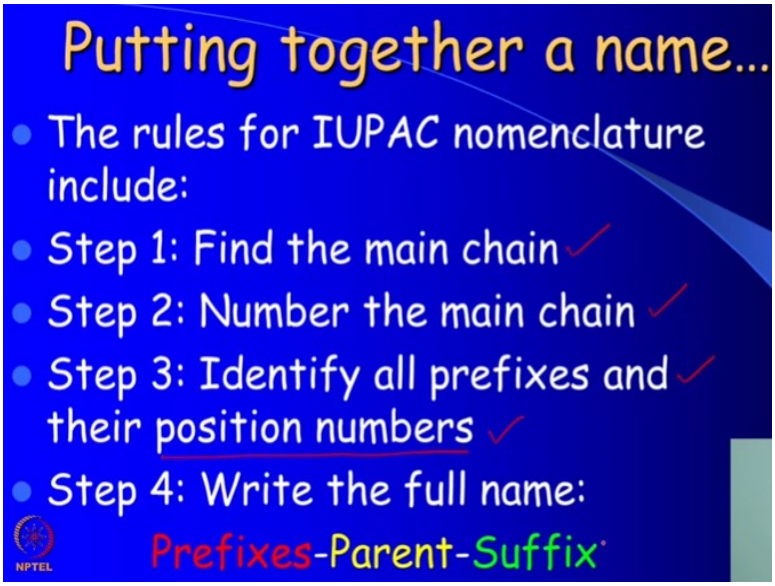

So the name of that molecule should be; first you must find out the main chain the number carbon atoms present in the main chain. You should identify the prefixes and their positions which is very important and then write the full name in a form of prefix, parent and suffix.

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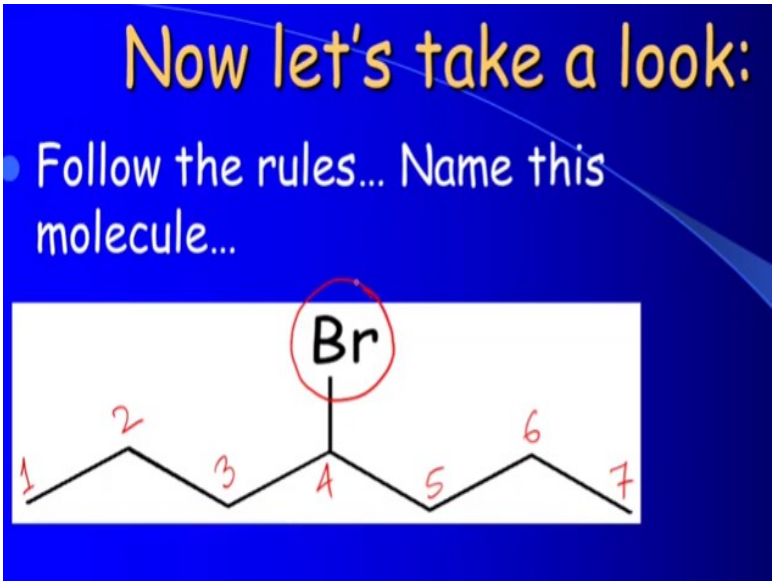

So if we go back to our molecule what do we see? We see here that this particular molecule has 1, 2, 3, 4, 5, 6, 7 carbon atoms so that means it is heptane and at 4 position you have a bromo substitution. So what should be the name of this compound?

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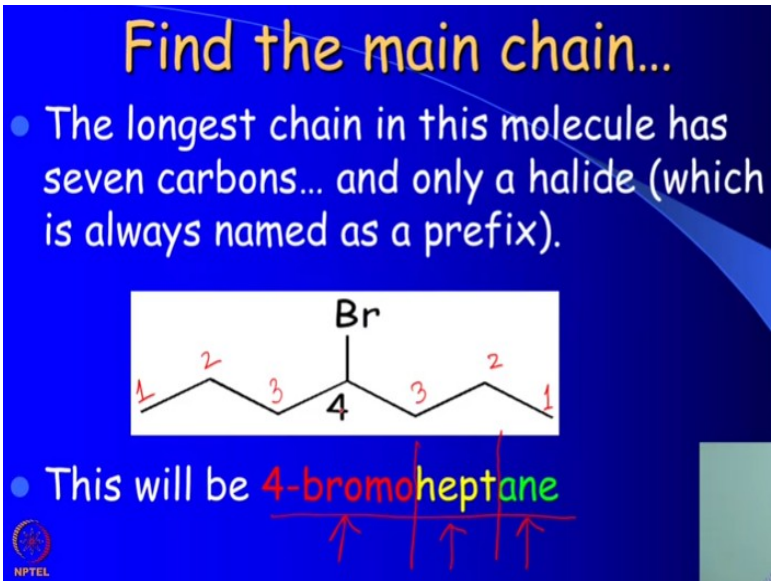

The name of this compound should be 4-bromoheptane what you can see is the first part that is written here is your prefix, then you have the parent and the suffix written in the appropriate color code. In this particular compound if you see if we try to number from the right this positive is 4, if you try to number from the left this position is again 4. So it does not matter from which side you number it is always written; the name is 4-bromoheptane.

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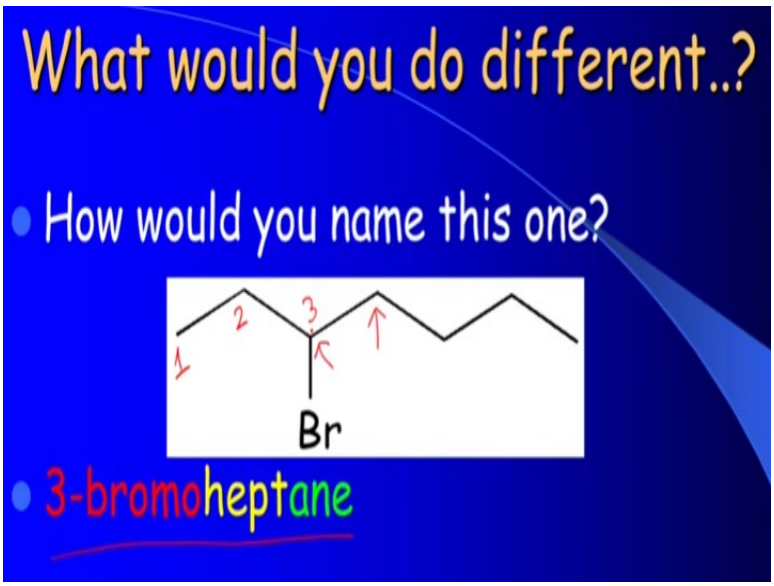

Let us see this the second molecule now you will see we have a very similar molecule which is also again a derivative of heptane, you have 7 carbon atoms here but you see this bromine is now shifted from the central position to this position. So now to write the name we should write the

name from the left hand side such that this carbon gets the lowest number. And in that way it is 1, 2, 3, so the name of the compound turns out to be 3-bromoheptane.

So here, it becomes important from which side of the chain you are numbering you should do the numbering from the side such that your prefix gets the lowest numbering in the long chain.

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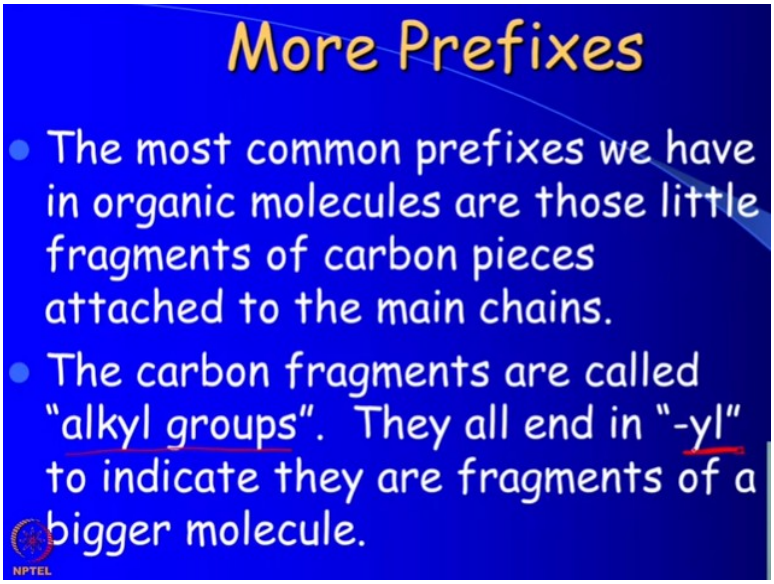

There are many different types of prefixes and those prefixes will have different types of names. So one can have an alkyl group as a prefix, alkyl group means a group containing 1, 2, 3 or more number of carbon atoms bonded to a longer chain. So when you have alkyl groups connected to a molecule in a chain you will add yl with the name of that alkane and then add that part in the front of the name of that particular compound.

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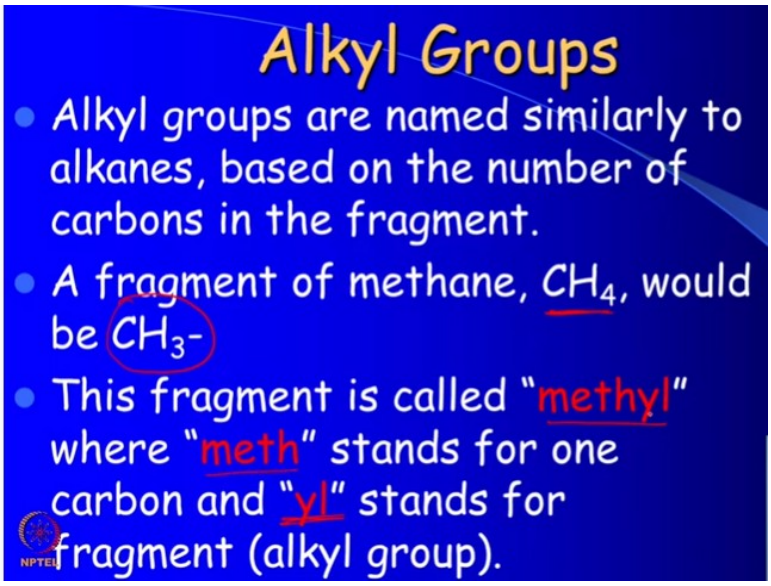

So when you have methyl group that is one carbon, that is when you have CH3. And then you write that CH3 group as a methyl group, originating from methane by removing 1 hydrogen you get a methyl group and this methyl group when it is connected to any long chain this yl is added against the meth. So it becomes methyl.

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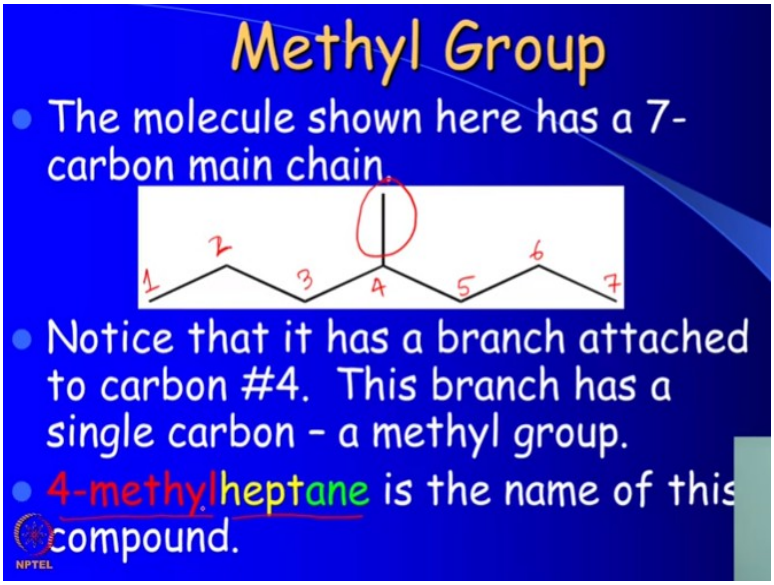

So in this particular compound we can now easily see that this methyl group which is attached here is again coming in the middle of the molecule. So we write the name of the molecule as usual heptane but here the prefix is 4-methyl.

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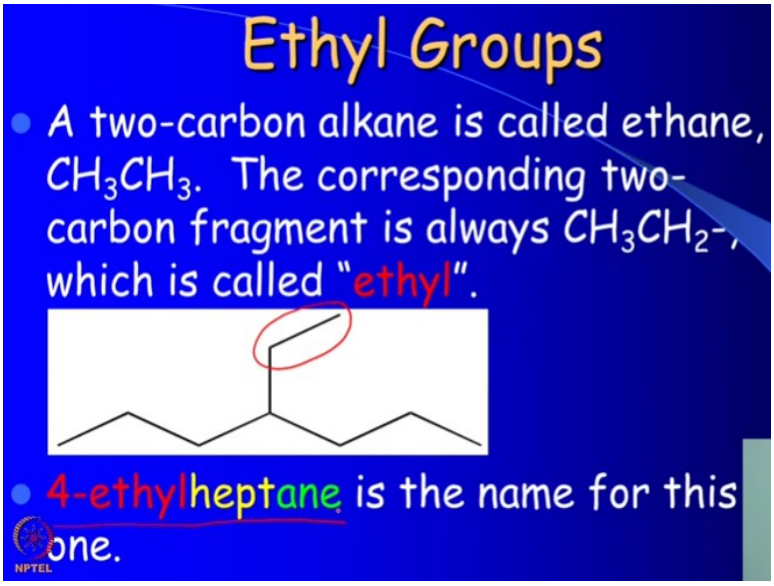

Then when you have an ethyl group which is a 2 carbon compound which is now attached at the same place like before. So we write the name of this compound as 4-ethylheptane. I hope you are able to follow this nomenclature methodology.

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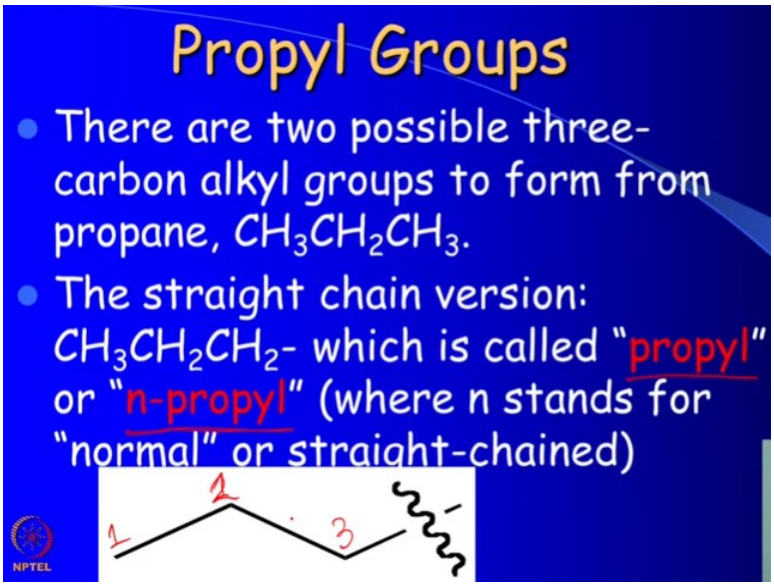

So when you have 3 carbons that are connected to a longer chain there are different possibilities. The first possibility is just a propyl group which we normally write as n-propyl group where those 3 carbons are connected in a row 1, 2 and 3. And these 3 carbon chain is bonded to a larger chain and we call it as n-propyl group.

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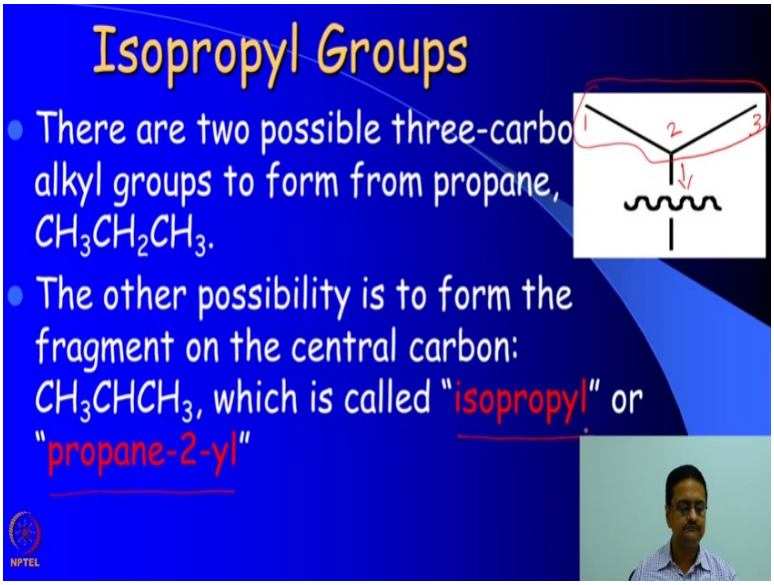

The propyl groups have other possibilities like isopropyl group where you have 3 carbons connected one after another. But the group of those that 3 carbons, is connected to the main chain to the middle carbon. So that particular compound will have a prefix of propane-2-yl or isopropyl group.

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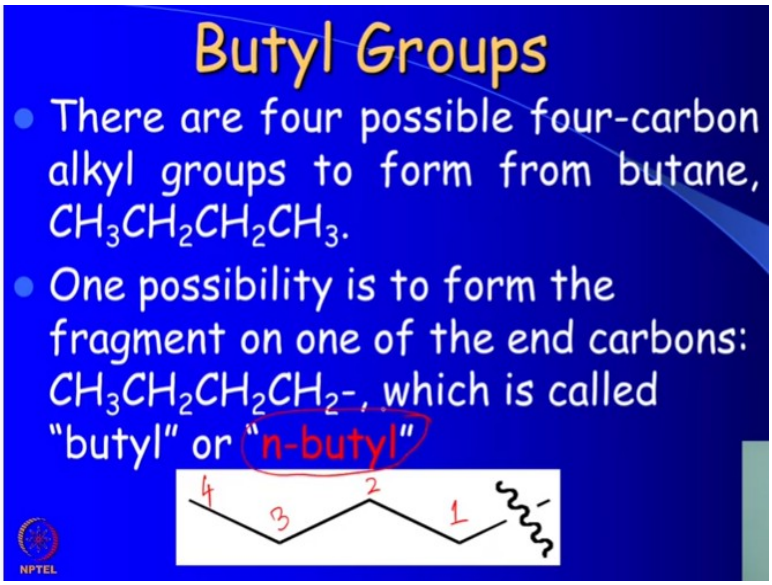

Then when, you have 4 carbons in a group that is called the butyl group or n-butyl group. And this n-butyl group also has different possibilities so in this particular representation you can see that the 4 atoms that are connected in a row is in turn connected to a longer chain. So we call this type of connectivity as n-butyl group.

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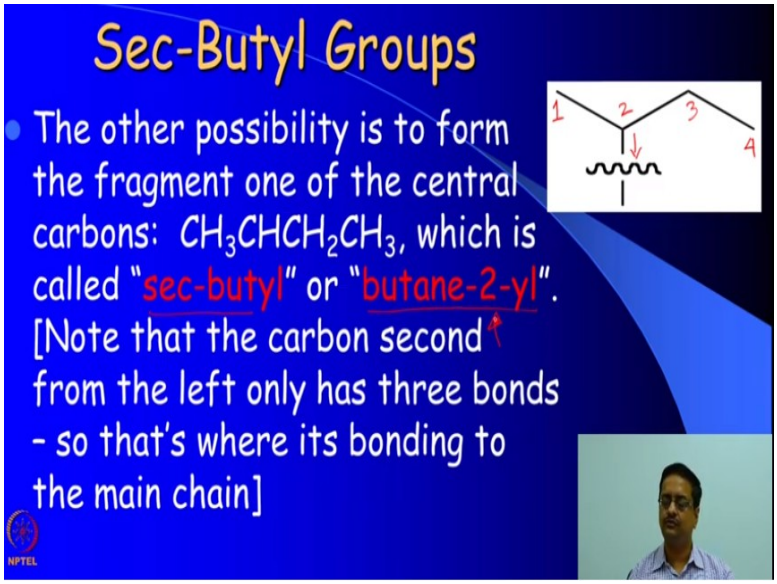

The other possibility of this butyl chain is called sec-butyl or secondary butyl group and that sec-butyl is written as butane-2-yl where you may see that this chain of 4 carbons 1, 2, 3 and 4 is connected to the main molecule through the position 2. And that second position is identified here and we write that, it is a butane-2-yl group that is connected to our main molecule.

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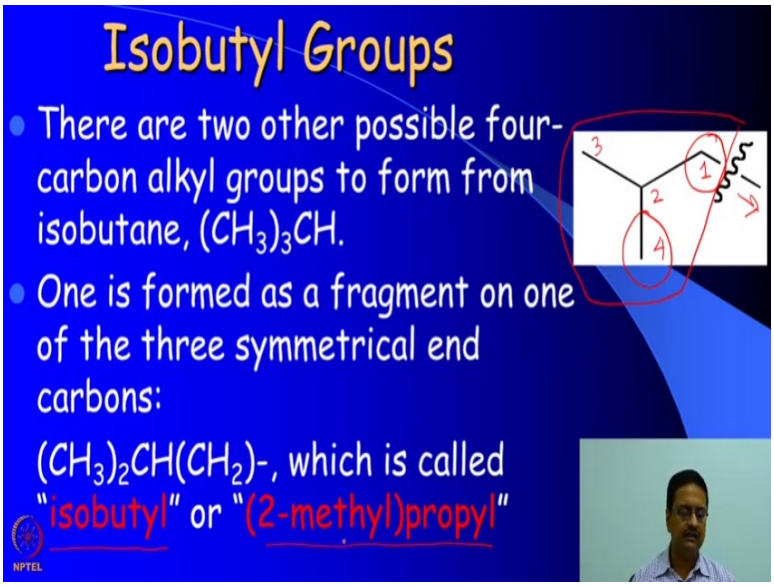

The other possibility is that it can be an isobutyl group where you can have a situation that the 4 carbon atoms are bonded like that and the connectivity of that part that fragment with the main chain is through this carbon atom. So this particular group is called iso-butyl group or it is called the (2-methyl) propyl group. So what we can write it as 1, 2, 3 at 2 position you have a methyl substitution. So we will separately name this group as a (2-methyl) propyl because at 2 position

you have a methyl and this is a propyl. So we can name it as a (2-methyl) propyl group that is attached to a larger chain.

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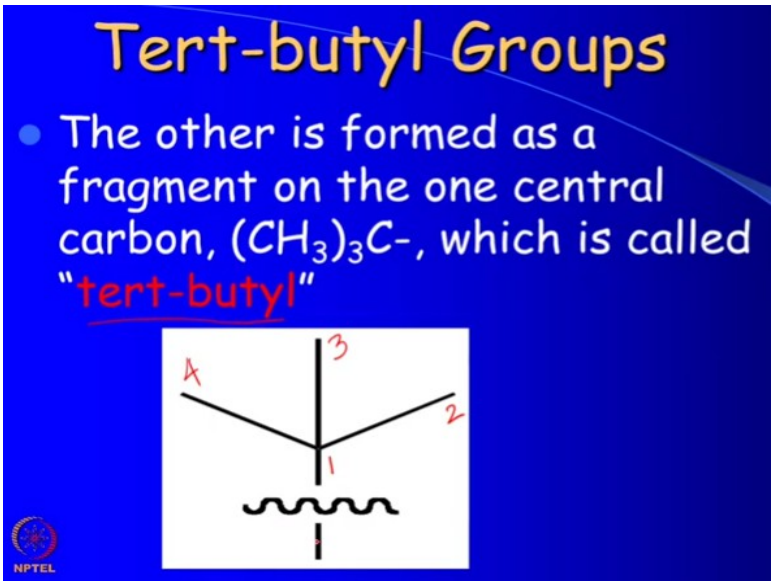

The last possibility having 4 carbon atoms it is called a tertiary butyl group or in short it is called a Tert-butyl groups where you have 4 carbon atoms bonded like that. So this carbon which does not have any hydrogen on it contains 3 carbon atoms and is bonded to the main chain is called a Tert-butyl group. So for a butyl group you see there are 4 different possibilities.

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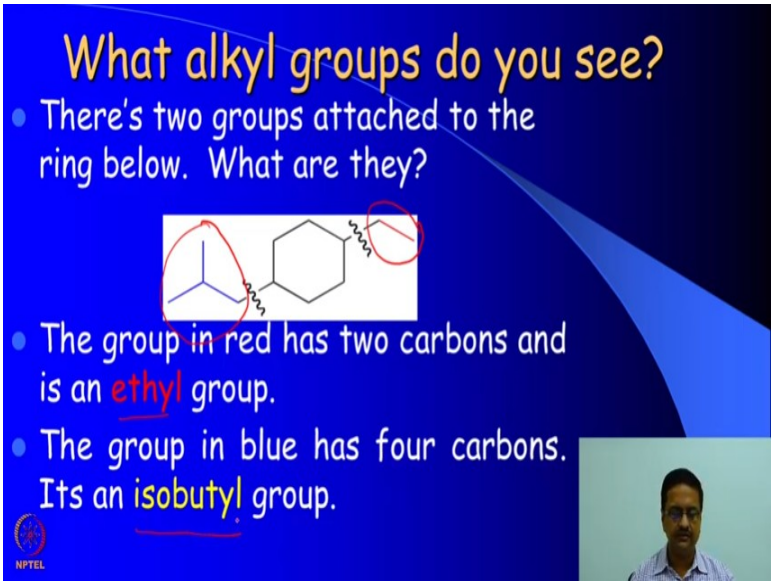

So now let us see what kind of groups that we see in this particular molecule. You see in the center what you see is a 6 membered ring this 6 membered ring is called cyclohexane because a

long 6 membered chain would be called hexane. And since it is a cyclic compound we write it as a cyclohexane. Now in this cyclohexane we have 1 ethyl group and here we have 1 isobutyl group so there are 2 alkyl groups connected to this molecule.

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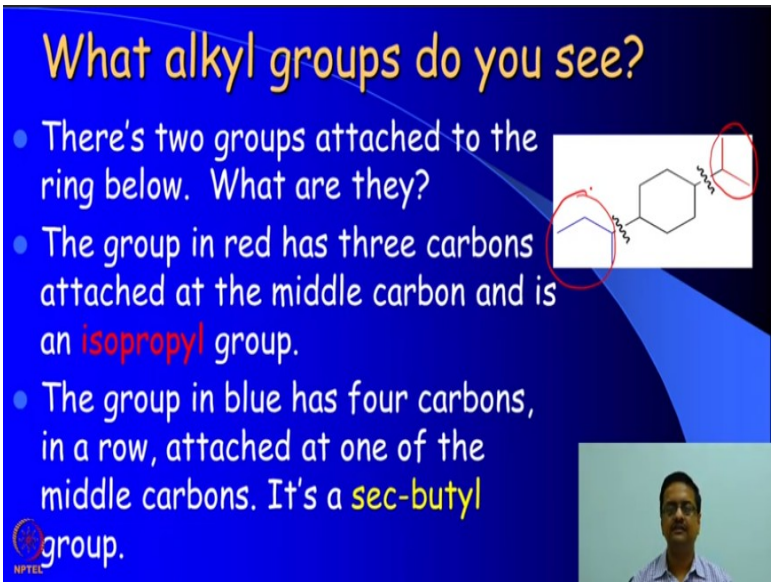

So when we have such things if there are 2 groups attached to the ring below what are those 2 here in this particular case? Here it is isopropyl group and there it is a sec-butyl group so this is very common that organic molecules can have multiple alkyl groups present and attached to the main ring or main chain.

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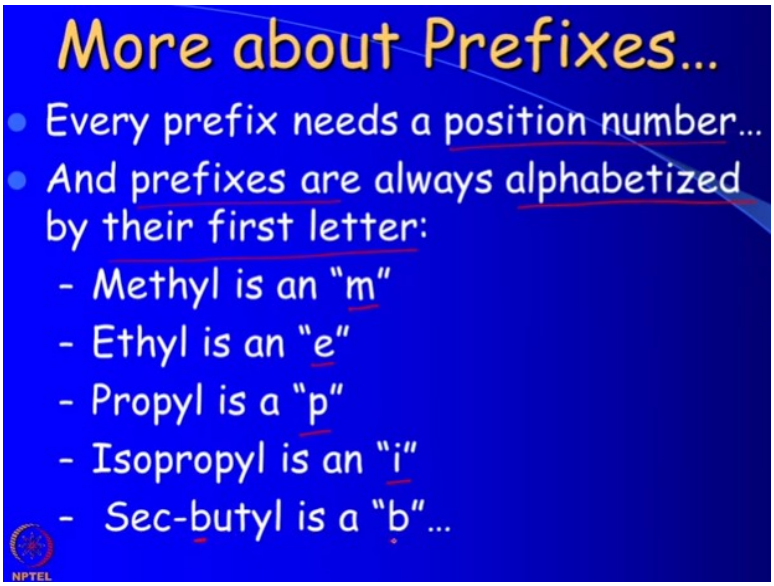

So when you talk about the prefixes we need to alphabetize those prefixes when we try to write their names. So every prefix needs a position number and the prefixes are always alphabetized with their first letter. So methyl is m, ethyl is e, propyl is p, isopropyl is i and sec-butyl we write it as b not as s.

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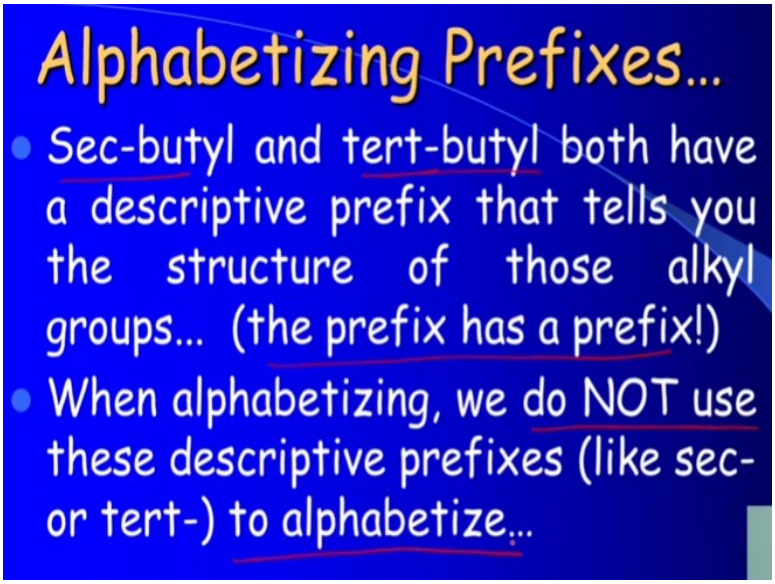

Why is that the sec-butyl and tert-butyl groups are coming from the same descriptive prefix that tells you the structure of those alkyl groups the prefix has a prefix. So when alphabetizing we do not use these descriptive prefixes like sec-butyl or tert-butyl to alphabetize. So we write them in a different way.

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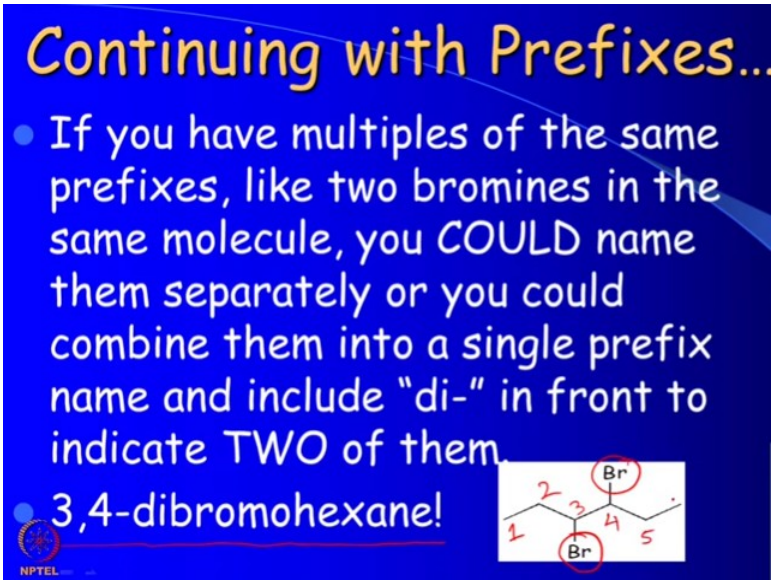

So if you have multiple of the same prefix for example in this particular case you have 2 bromo compounds you could name them separately or you could combine into a single prefix and name them as a di- in front of it. So in this particular case we write it as 3, 4 dibromohexane as you could see this contains 6 carbon atoms.

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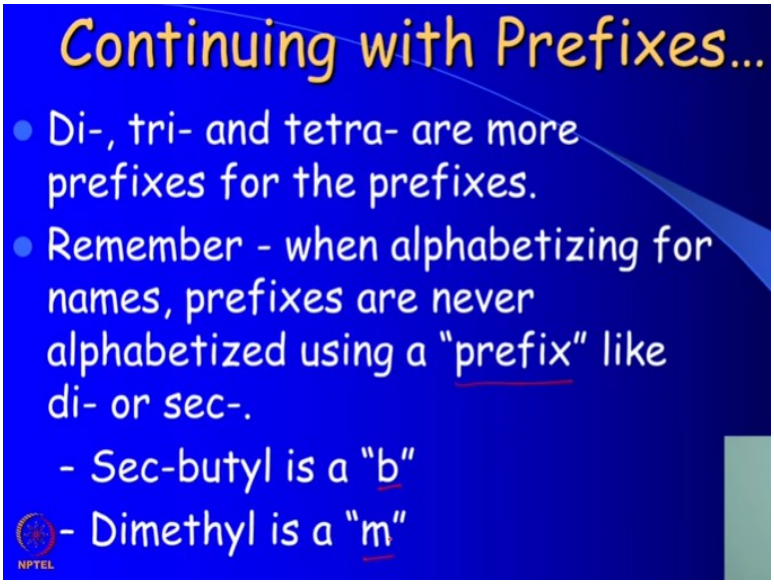

So you can have di, tri, tetra, pent etc., as your prefixes remember when the alphabetizing for the names prefixes are never alphabetizes using another prefix. So sec-butyl is b and dimethyl it is written as m and that is how it is alphabetized.

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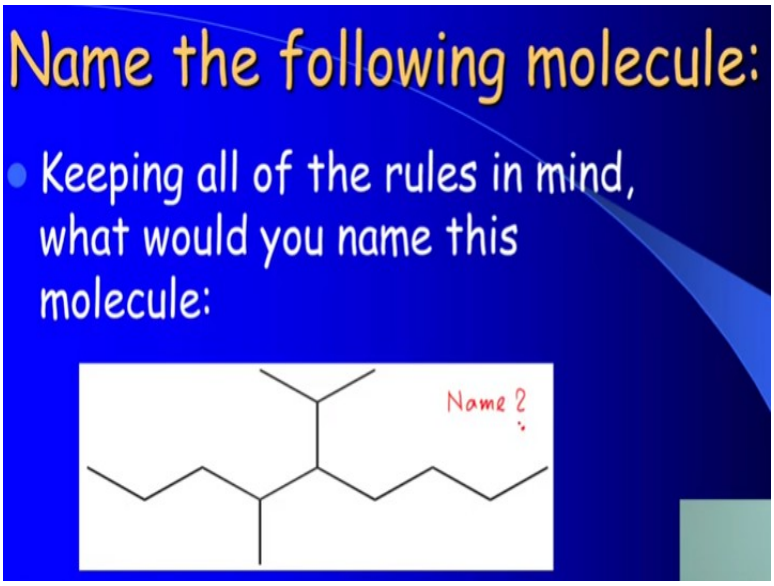

So now I would like you to name this particular compound this is the first homework of your course where I would like you to identify the name of this molecule following the IUPAC nomenclature method. So we will continue the next lecture from this point but this is your first homework of this course.