



Survey of Organic Chemistry and Biochemistry Handout 1.2 Alkanes, Part 1

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From our previous lesson we learned about hydrocarbons. **Hydrocarbons** are organic compounds composed of only **carbon** and **hydrogen**. We looked at four functional groups that fall into this category: alkanes, alkenes, alkynes, and aromatic (arenes).

**Please note that if you are reading both the handouts for Survey of Orgo and my Orgo for Health and Life Sciences, I will refer to aromatic hydrocarbons as aromatics in these sets of handouts (for survey) and as arenes (for orgo for health/life sci). They are the same.

In this lesson, we will focus on **alkanes**, which are hydrocarbons containing only **single bonds**.

In an example from Handout 1.1, we looked at methane, CH_4 . Since carbon is tetravalent, it forms four bonds. So now we will see what happens when there are 2, 3, 4...etc. carbons in the organic compound.

The general formula for alkanes is $\text{C}_n\text{H}_{2n+2}$.

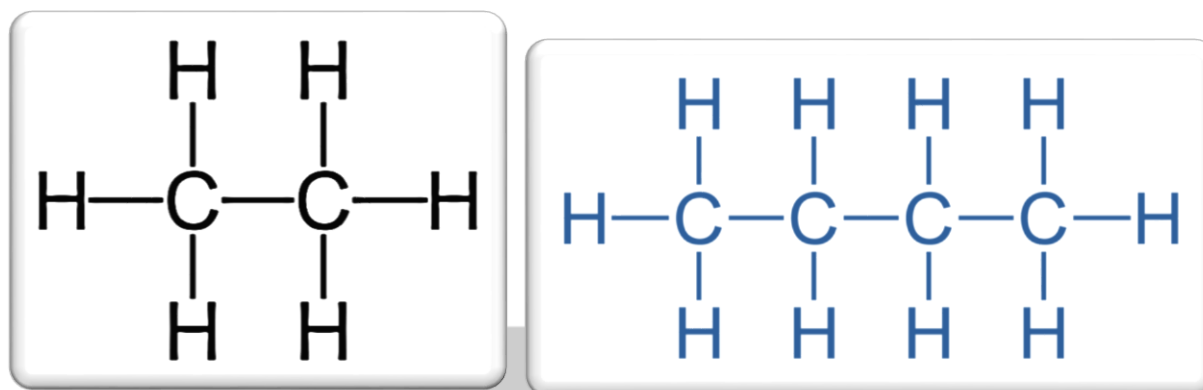
Let's look at methane. There is one carbon ($n = 1$). For hydrogen, we plug in "1" to the equation $2n+2$ to get $2(1) + 2 = (2 + 2) = 4$.

The next one is ethane which has 2 carbons and 6 hydrogens: let $n = 2$, number of hydrogens is $2(2) + 2 = (4 + 2) = 6$
(Don't worry it's not going to go into calculus! I have separate handouts for that.)

For hydrocarbons (alkanes, alkenes, alkynes, aromatics), the rule is that each carbon MUST be bonded to another carbon. When we draw the figures for alkanes, you will be able to visualize it.

Examples: Ethane, C_2H_6 and Butane, C_4H_{10}

Figures 1 and 2 - Ethane, C₂H₆ (left) and Butane C₄H₁₀ (right)



As the number of carbons and hydrogens increase, molecules can be formed in different ways. They can be **straight-chain alkanes** or **branched-chain alkanes**.

For example, C₄H₁₀ can be formed in two ways. Let's begin by taking a look at our example above: Butane, C₄H₁₀

Straight-chain alkanes are what the name states. They are alkanes that are connected in a continuous, straight line. An example would be butane from Figure 2 above.

Branched-chain alkanes have a branch point where the carbon forms a branching connection (similar to the branches of a tree). An example would be 2-Methylpropane.

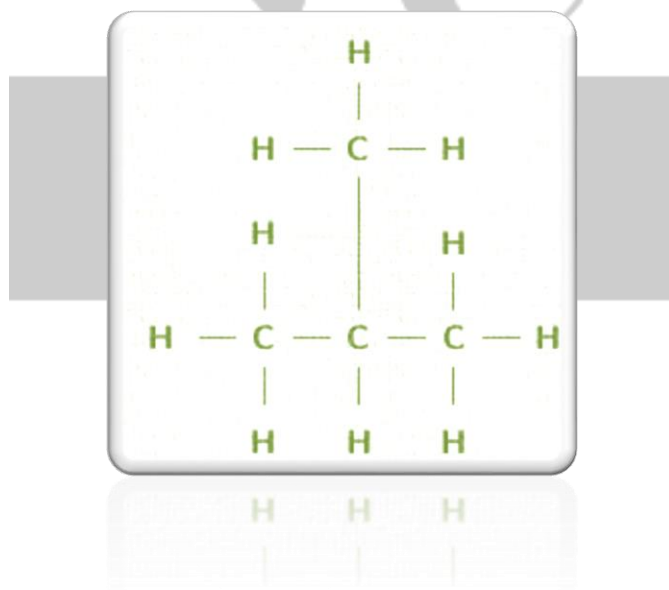


Figure 3 - 2-Methylpropane

For straight-chain alkanes, you can move your finger across the line of carbons without having to lift it or retracing your path. However for branched-chain alkanes, you will have to either lift your finger or retrace your path (if you decide to not lift your finger from the page).

This brings us to our next point- **isomers**. **Isomers** are molecules with the same chemical formula (such as our two examples butane and 2-methylpropane), but have different chemical structures.

Specifically, **constitutional isomers** are compounds that have the same chemical formula, but have different connections/connectivity among their atoms.

Although isomers have the same chemical formula, they have different physical and chemical properties. Their structures are different and can have different physiological effects and properties.

For example, boiling point and melting point. Butane has a boiling point of -0.5°C while 2-methylpropane has a lower boiling point of -11.7°C . This is due to butane having greater dispersion forces since it's flatter and less compact. But for survey of orgo, you just need to know that isomers have different properties despite similar chemical formulas.

Condensed Structures

From Figures 1 through 3, we drew the structures for ethane, butane, and 2-methylpropane. Although it is useful, it can take a lot of time. A simpler and more organized way to draw these structures are through condensed structures. In **condensed structures**, the connections between atoms are understood while providing the necessary information such as which functional groups are present.

Remember our review of the number of bonds that the elements can form from the table of Handout 1.1? These will help us interpret condensed structures more easily as we move on.

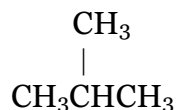
	Group Number	Valence Electrons	Number of bonds it can form
Hydrogen	1A (1)	1	1
Nitrogen	5A (15)	5	3
Oxygen	6A (16)	6	2
Fluorine, Chlorine, Bromine, Iodine	7A (17)	7	1

Let's take a look at the condensed structures for ethane, butane, and 2-methylpropane.

Ethane: CH_3CH_3

Butane: $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$

2-Methylpropane:



Instead of putting the lines representing the bonds, we can assume their connections from the condensed structures. It won't be a problem to draw out the entire structure for simple organic compounds (such as our examples), but later on when we get to larger organic molecules with many connections, it will be very difficult and messy to draw out the entire structure.

Condensed structures will be very helpful when we start drawing and naming organic compounds.

In our above example for 2-methylpropane, the vertical bond with the second carbon is shown to clarify the structure. We will see how helpful this is when we try to visualize isomers with similar chemical formulas.

Another way to simplify condensed structures is through parentheses. Let's take a look at pentane, C_5H_{12} :

The condensed structure for pentane is $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$

We can further simplify this by writing: $\text{CH}_3(\text{CH}_2)_3\text{CH}_3$

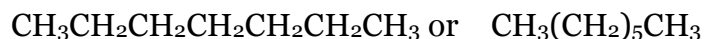
Isn't that much easier and cleaner to read?

The subscript tells us how many of the CH_2 bonds there are between the two CH_3 bonds.

Now that we have a foundation for drawing and identifying straight-chain and branched-chain isomers of organic compounds, let's apply this to an example.

Example: Draw the straight-chain and at least three (3) branched-chain isomers with the formula C_7H_{16} .

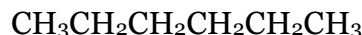
The straight-chain isomer with the formula C_7H_{16} is



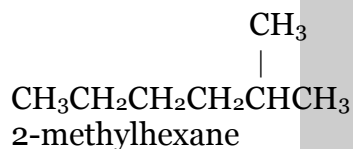
The branched-chain isomers can get a little more complicated; however, it's not too bad, I promise!

Step 1:

What I usually did was first subtract one carbon from the chain and then attach it to the second or second to the last carbon in the straight chain. Here's what we will have after subtracting and before attaching:

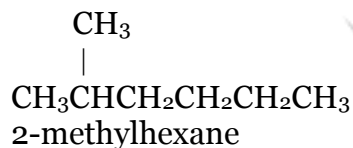


After attachment to the second to the last carbon, we get:



You can also start from the left and it will still be 2-methylhexane. We will learn about this when we discuss conformers next. When we learn how to name alkanes (as well as other organic compounds), we will see that they will be the same as a result of identical connections. For now we'll just take a look at the branched isomers.

Let's flip it around and we get:

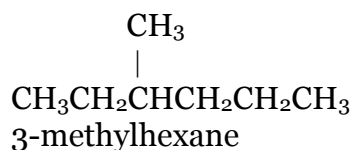


In our example above, the new chain I would draw would have six (6) carbons. If you attach the carbon to the first carbon or the last carbon of the chain, you will end up with the same straight-chain isomer with seven carbons forming a linear row.

Next we can put the methyl group (the $-\text{CH}_3$) in the middle. We will learn about substituents ($-\text{CH}_3$, $-\text{CH}_2\text{CH}_3$, etc.) after we finish this exercise. I know what you're thinking...it's only the beginning of orgo and there's already so much information to take in!

Don't panic if it seems like a lot. It will click once we get through this handout. Like I said before, it took me time also to be familiar with orgo when I was an undergraduate student so don't feel any pressure to have to know all of this right away.

Back to our example, let's add the methyl group ($-\text{CH}_3$) to the third carbon:

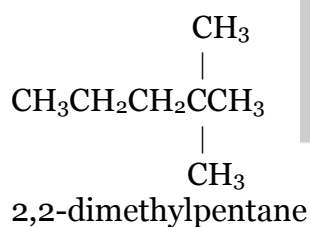


Step 2:

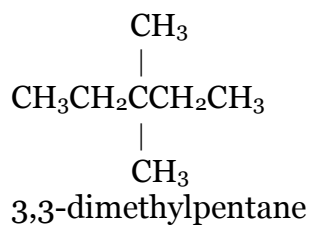
Continue now and take away two carbons and form a five carbon chain. We get:



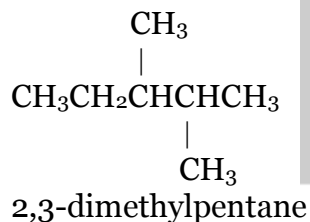
We continue again and branch them from the carbons to the second or second to the last carbons in the chain.



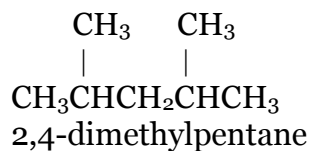
If we put them in the middle (the third carbon):



If we put them in the second and third carbons of the five carbon chain:



We continue looking for different connections:



You just need to memorize the first four in terms of names. However if you want a mnemonic, I used “**Mom Eats Peanut Butter**”. (Yes I loved food when I was an undergrad so many of my mnemonics were related to food!)

For pentane through decane, they follow the Greek numbers. I’m sure all of you are familiar with this from the polygons from geometry with pentagon, hexagon, heptagon, octagon, nonagon, and decagon.

The organic chemistry nomenclature (the naming system) that is in use today was formulated by the International Union of Pure and Applied Chemistry (IUPAC).

According to the IUPAC’s system for naming organic compounds, the chemical name is composed of three parts based on the longest continuous chain:

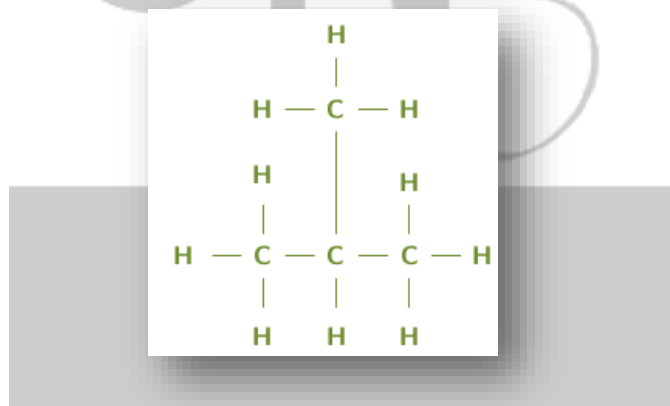
Prefix- the location of the substituents and functional groups in the molecule

Parent- the number of carbon atoms

Suffix- the family a molecule belongs to

(**Locant** will also be discussed in my Orgo for Bio/Life Sci, but don’t worry about it for now because we can combine it with prefix. It’s basically the position of the substituent in the chain specified by a number. In 2-methylpropane, “2” is the locant since it’s branched from the second carbon on the main chain.)

Let’s reexamine our example from Figure 3: 2-methylpropane.



We will do naming step by step next, but for reference now, it should be easy to follow in this example.

Prefix:

As I had discussed earlier, the methyl group is the -CH_3 substituent. For the prefix, we need to know the location and what type of substituent it is.

In this case, the methyl group branches off from the second carbon (the longest chain). You will see that regardless of which carbon you choose (left, right, or top), the methyl group will always be on the second carbon. We have “**2-methyl.**”

Parent:

The parent is the number of carbons on the longest chain. In this case, three carbons are our longest chain so the parent begins with “**prop-**”

Suffix:

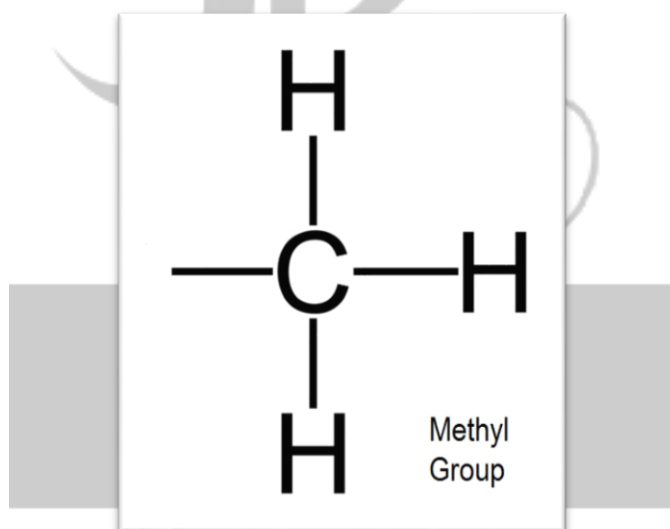
Finally we classify it based on its family. Remember the functional groups handout that accompanied Handout 1.1? When we look at it again we see that alkanes end in “**-ane**”.

Put it all together and we get 2-methylpropane. We named our first organic compound!

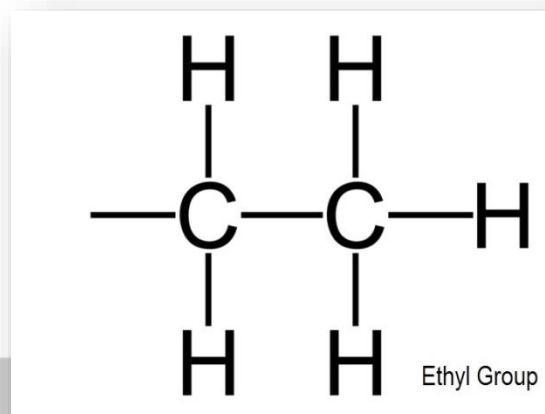
I highlighted in our recent example that the methyl group is a substituent.

Substituents are atoms or groups of atoms attached to the parent compound. Now we will learn how we got $-\text{CH}_3$, $-\text{CH}_2\text{CH}_3$, etc. which are called alkyl groups.

Alkyl groups are derived from a parent alkane. A hydrogen is removed to allow for bonding. If we remove the hydrogen from methane (CH_4) to create a bonding site, we get $-\text{CH}_3$. The $-\text{CH}_3$ alkyl group is known as the methyl group.

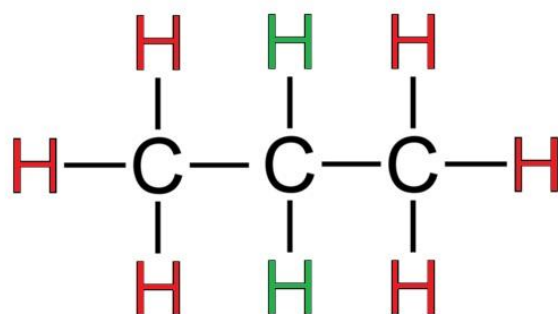


We can also do this for ethane to create the ethyl group ($-\text{CH}_2\text{CH}_3$). We remove the hydrogen and get:



As you can see from our examples, to name an alkyl group remove the **-ane** suffix and replace it with **-yl**.

It's simple for methane and ethane because regardless of which hydrogen you remove, there will only be one possible type of methyl or ethyl group. However, once we move to propyl, a removal of the hydrogen can yield two different alkyl groups.



Propane, C₃H₈ (or CH₃CH₂CH₃)

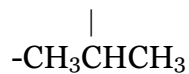
We can see from the diagram that there are two types of hydrogens that you can remove: a hydrogen attached to the ends (red) or a hydrogen in the middle (green).

If you remove a hydrogen from the ends (it won't matter which of six you choose), you will get:



This is known as the **propyl group** (or n-propyl for normal) which is a straight chain alkyl group. However it is assumed that propyl (with an absence of a prefix) is the straight chain without having to add n-.

If you remove a hydrogen from the middle (one of the two), you will get:



This is known as the isopropyl group (the branched chain alkyl group). You can also write it as a condensed structure with parentheses as $(\text{CH}_3)_2\text{CH}-$.

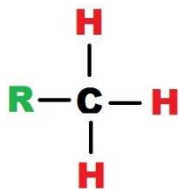
Here are some common alkyl groups that you will encounter:

$-\text{CH}_3$	$-\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$
Methyl	Butyl (n-butyl)
$-\text{CH}_2\text{CH}_3$	$\begin{array}{c} \\ \text{CH}_3\text{CHCH}_2\text{CH}_3 \end{array}$
Ethyl	sec-Butyl
$-\text{CH}_2\text{CH}_2\text{CH}_3$	$\begin{array}{c} \text{CH}_3 \\ \\ -\text{CH}_2\text{CHCH}_3 \end{array}$
Propyl (n-propyl)	Isobutyl
$\begin{array}{c} \\ \text{CH}_3\text{CHCH}_3 \end{array}$	$\begin{array}{c} \\ \text{CH}_3\text{CCH}_3 \\ \\ \text{CH}_3 \end{array}$
Isopropyl	tert-Butyl

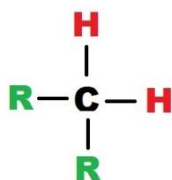
From our table we were introduced to sec- (which stands for secondary) and tert- (which stands for tertiary). These refer to the number of other carbons attached to the branch point. For secondary, two carbons are connected to the carbon branch point. For tertiary, three carbons are connected to the carbon branch point.

Carbon has four possible substitution patterns: **Primary (1°)**, **secondary (2°)**, **tertiary (3°)**, and **quaternary (4°)**.

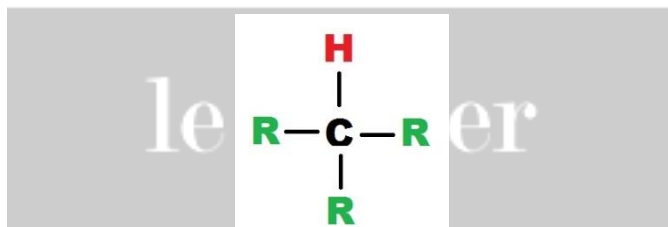
A primary carbon atom has one other carbon atom attached to it:



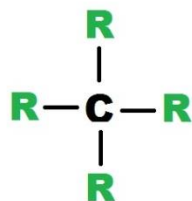
A secondary carbon atom has two other carbons atoms attached to it:



A tertiary carbon atom has three other carbon atoms attached to it:



A quaternary carbon atom has four other carbon atoms attached to it:

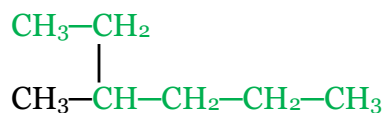


Diagrams of carbon's possible substitution (where **R** = the alkyl group for our examples here; however, in later examples, **R** = any organic substituent). Please take a look at the functional groups worksheet. For an alkyl halide, **R-X** would be the general formula and can represent CH_3Cl (chloromethane or methyl chloride), $\text{CH}_3\text{CH}_2\text{Cl}$ (chloroethane or ethyl chloride), etc.

Naming Alkanes: Methods

Here's where we learn how to name branched alkanes.

- 1. Find the longest carbon chain and name it according to the number of carbons it has. Make sure you count ALL of the chains since it might not be as obvious.**

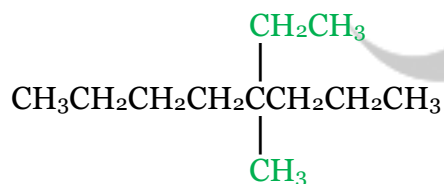


The longest chain would be a substituted hexane, not pentane. It's easy to make a mistake by counting from left to right and getting pentane. This would mess up the naming since counting from left to right from the five carbon chain would name "2-ethylpentane" which is wrong.

Counting correctly from the longest six carbon chain would give you "3-methylhexane."

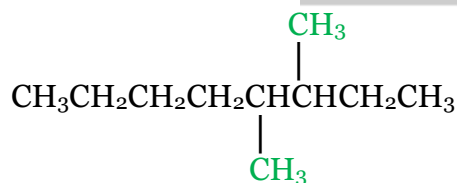
2. Number the carbon atoms in the main chain according to the nearest branch point (giving the lower number). In our example, the branch point would be on carbon 3. If you started from the right, you would get "4-methylhexane." Although you got the methyl and the hexane right, the locant (position of the substituent) is wrong.

3. If there are two substituents attached to the same carbon, BOTH of them must be assigned a number. The two different substituents are listed in alphabetical order (for example, ethyl comes before methyl). Numbers are separated from words through dashes.

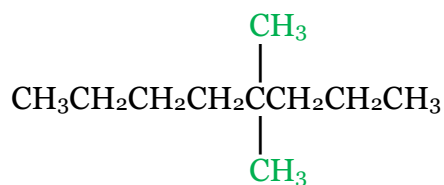


4-ethyl-4-methyloctane

4. Combine everything into a single word (prefix, parent, and suffix). If there are identical substituents in the chain, the prefixes di-, tri-, tetra-, etc. are used. Numbers are separated by commas. And remember that numbers and words are separated by dashes.



3,4-dimethyloctane



4,4-dimethyloctane

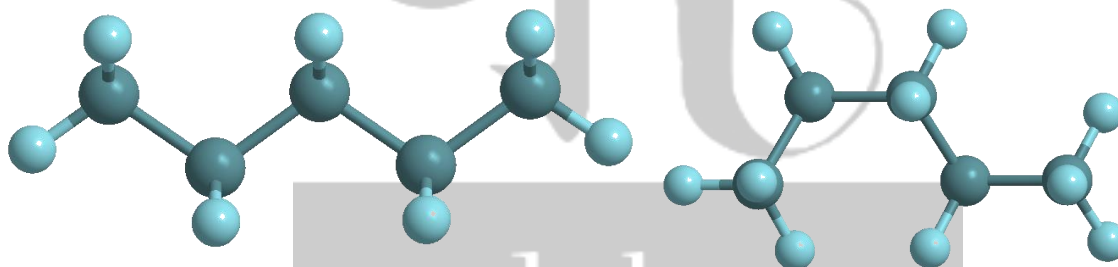
Organic Molecule Shapes

We will briefly discuss conformation and conformers. A more in depth discussion on conformation/bond rotation will be in my organic chemistry for health and life sciences handouts. That information, however, is beyond the scope of the survey of orgo notes.

We saw the structures of many organic compounds and their isomers through their condensed structures above. However, they do not address their geometry, only the connections between atoms. Remember from our first handout that carbon is tetravalent and forms four bonds.

The three dimensional arrangement of the carbon-carbon single bonds gives rise to an infinite number as a result of rotation happening around the carbon-carbon bonds. The infinite number of possible three dimensional geometries are called **conformations**.

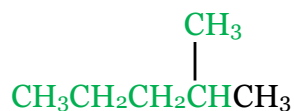
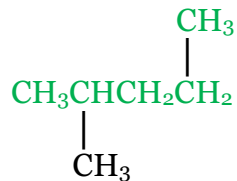
Let's take a look at two conformations of pentane:



This states that there is constant change with regards to the shape of the molecules at any moment. However, at any given instant, most of the molecules are in the least crowded, extended conformation (the left one in our example of pentane).

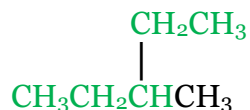
As long as the connections are similar between atoms in a structure, they represent the same compound regardless of how you draw it. These molecular structures are called **conformers**.

Let's take a look at an example:



When we look at the two compounds, we see that they have the same molecular formula, C_6H_{14} . Now that we verified that, we can count the longest chain and identify the substituent. They are both 2-methylpentane! They are identical to each other so they are **conformers**.

What if we look at this compound:



The molecular formula is the same (C_6H_{14}), but the substituent is located in a different carbon. While it was in the second carbon above, it's located on the third carbon here. Here we have 3-methylpentane. It is an **isomer**, not a conformer.

We covered a lot in this handout. I don't want to overwhelm you with material, so I will save the rest for Part 2 which will cover properties and reactions of alkanes (combustion and halogenation). We will then look at cycloalkanes and do a few more examples.

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