Naming Alkanes

This handout will:

- Define alkanes
- Show and explain how to name various alkanes

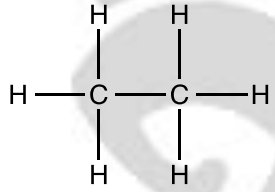
Introduction:

Alkanes are molecules that consist of only carbon and hydrogen atoms, all connected by single bonds. Names of alkanes change depending on how many carbons are in them, and in turn, how many hydrogens are attached to those carbons.

The general formula for an alkane is:

$$C_nH_{2n+2}$$

The **n** represents the number of carbons that are present. For example:



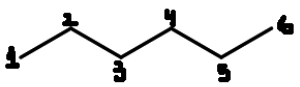
This molecule has 2 carbons, and we can see that it has 6 hydrogens just by counting them. Let's put these numbers into the formula we have to check that it works.

Our **n** in this case is 2. This gives us $C_2H_{2(2)+2}$, which simplifies to C_2H_6 Therefore we can confirm that the formula works.

Structural Formula vs. Stick Structures:

There are two different ways to draw alkanes. The molecule above was drawn as the **structural formula.** Another way to draw the same molecule is as a **stick structure.** Each stick represents two carbons, one at each end. The hydrogens are not drawn because they are assumed to already be there.

- **Example**: C_6H_{14}



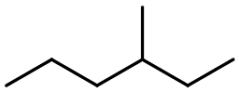
Names of Alkanes:

As mentioned prior, naming alkanes depends on how many carbons are present. Here is a table of names for alkanes containing 1 though 12 carbons.

n	Name	Formula
1	Methane	CH_4
2	Ethane	CH_3CH_3
3	Propane	$CH_3CH_2CH_3$
4	Butane	$CH_3CH_2CH_2CH_3$
5	Pentane	$CH_3(CH_2)_3CH_3$
6	Hexane	$CH_3(CH_2)_4CH_3$
7	Heptane	$CH_3(CH_2)_5CH_3$
8	Octane	$CH_3(CH_2)_6CH_3$
9	Nonane	$CH_3(CH_2)_7CH_3$
10	Decane	$CH_3(CH_2)_8CH_3$
11	Undecane	$CH_3(CH_2)_9CH_3$
12	Dodecane	$CH_3(CH_2)_{10}CH_3$

Sometimes, these alkane chains have a **substituent** in place of one of the hydrogens. A **substituent** is a carbon group, branching from the original carbon backbone. To name a substituent, you have to replace the ending *–ane* with *–yl*.

- **Example:**



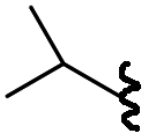
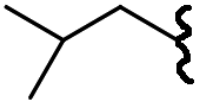
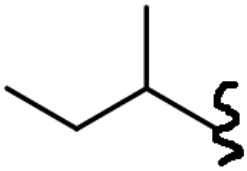
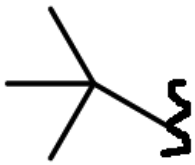
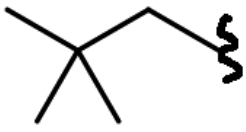
In this molecule, there is one substituent coming off of the carbon backbone. The substituent is made up of only one carbon, therefore instead of saying that we have a meth*ane* substituent, we call it meth*yl*. But how do you name a substituent that is branched, just like this one?

Naming of Substituents:

There are two naming systems that are used in organic chemistry: the **common name** and the **IUPAC name**. IUPAC naming literally describes the structure of the

subsituent, whereas the common name is more widely used in the world of organic chemisty. It's another way to describe the subsituent.

- **Example**: Let's take a look at isopropyl, which you can find in the table below. Isopropyl is named so because it is an isolated propyl molecule, made up of three carbons. It is also called 1-methylethyl because if we look at the substituent as it's own molecule, just for the time being, we can see that the longest carbon chain is an ethyl, and there is a methyl coming off of the first carbon. The reason we say that we have an ethyl chain is because there are two carbons, therefore we know it will be an ethane. But remember, we have to change the ending from *–ane* to *–yl*, so instead of ethane, we say ethyl. Same thing happens to methyl.

Branched Substituent	**Common Name**	**IUPAC Name**
	Isopropyl	1-methylethyl
	Isobutyl	2-methylpropyl
	Sec-butyl	1-methylpropyl
	Tert-butyl	1,1-dimethylethyl
	Neopentyl	2,2-dimethylpropyl

Since we are focusing on naming the substituents right now, the squiggly line represents the rest of the molecule that the substiteunt could be attached to.

Alkyl Halides:

A halogen is also treated as a substituent when it comes to naming alkanes. When it comes to halogens, you have to change the ending *–ine* to *–o*. If you have fluorine coming off of the carbon chain, it is named as *fluoro*. Same thing goes for chlorine, bromine, and iodine. They would be called brom*o*, chlor*o*, and iod*o* respectively.

Rules to Name Alkanes:

Remember that to name substituents, you have to change the ending of the subsituent depending on how many carbons it consists of, or what halogen it is. If it is a branched subsituent, the common name or the IUPAC name is used, both of which are presented in the table on page 3.

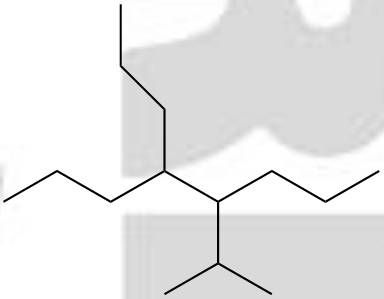
So now that you know how to name an alkane chain as well as how to name any substituents that may be included, there are a set of rules that should be followed when you name alkanes. These rules were created in order to provide a logical and systematic way to name alkanes, and to prevent confusion.

Naming Rules:

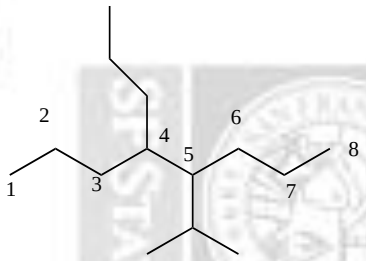
1. Find the logest chain of carbons in the molecule and name it.
2. Name all the groups attached to the longest chain as alkyl substituents.
3. Number the carbons of the longest chain, beginning with the end closest to a substituent.
4. Write the name of the alkane by arranging all the substituents in alphabetical order.

Let's look at an example and use the rules one by one to name our alkane.

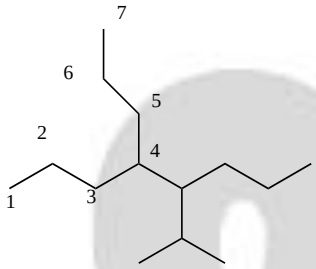
Example 1: Name this molecule.



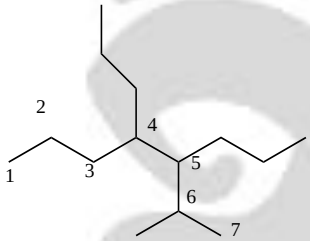
- **First**, find the longest chain of carbons in the molecule and name it. Let's start from the left-most carbon and count to the right. It looks like we have 8 carbons in that chain.



What about if we started from the left most carbon and counted upwards? In that chain, we have only 7 carbons.

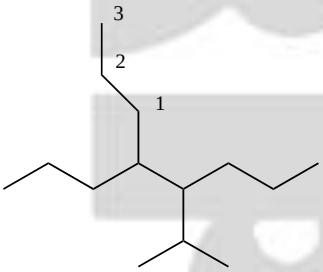


What about if we still started from the left and counted down? Still only 7 carbons.

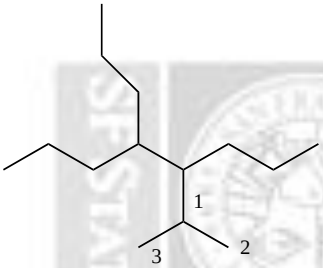


The longest chain of carbons here is the chain with 8 carbons, and this is called **octane**.

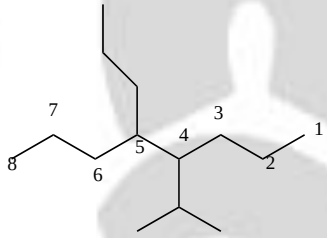
- **Second**, name all the groups attached to the longest chain as alkyl substituents. Let's name all the groups that are attached to our octane carbon chain. Starting from the group closest to the left, it looks like we have a 3-carbon chain attached to our molecule. What is that called? A propane! But, in this case, it will be called **propyl** because it is an attached substituent.



The other group we have is the one closest to the right. What do we call a group that starts with a carbon, that is attached to two other carbons? An **isopropyl *or* 1-methylethyl!**

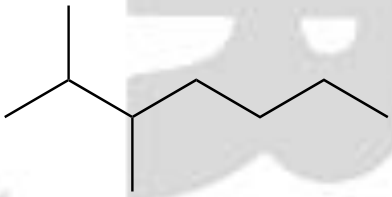


- **Third**, number the carbons of the longest chain beginning with the end closest to a substituent. We have two substituents in our molecule, a propyl and an isopropyl. Which one is closest to the end of the chain? It looks like both of the substituents are coming off of the 4th carbon. When you have a case like this, you have to choose the side closest to the substituent that comes first in the alphabet. Between an isopropyl and a propyl, the isopropyl comes first, so we start numbering from the right side.

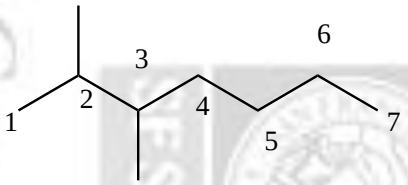


- **Finally**, write the name of the alkane by arranging all the substituents in alphabetical order. We know that we have an **octane** chain, we have an **isopropyl** attached to the **4th** carbon, and we have a **propyl** attached to the **5th** carbon. When you arrange all the substiuents in alphabetical order make sure to put the carbon number to which it is attached along with a dash. Arranging all the substitunets in alphabetical order, we get **4-isopropyl-5-propyloctane** or alternatively **4-(1-methylethyl)-5-propyloctane.**

Example 2: Name this molecule.



- First, find the longest chain of carbons in the molecule and name it. Our longest chain has 7 carbons. That's called a **heptane**.
- Name all the groups attached to the longest chain as alkyl substituents. Here, we just have two methyl groups.
- Then, number the carbons of the longest chain, beginning with the end closest to a substituent.



- Lastly, write the name of the alkane by arrnaging all the substituents in alphabetical order.
- We get, 2,3-dimethylheptane as our answer.

Citations

ChemDraw. (n.d.). Retrieved December 2, 2014, from http://www.cambridgesoft.com/Ensemble_for_Chemistry/ChemDraw/

Chemical Structure Drawing Search - eMolecules. (n.d.). Retrieved December 2, 2014, from https://www.emolecules.com

Vollhardt, K., & Schore, N. (2007). *Organic Chemistry* (5th ed.). New York: W.H. Freeman and Company.