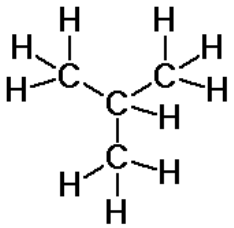
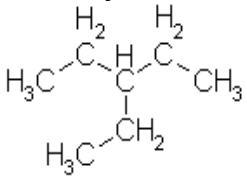
2.2 Naming of Alkanes

Frequently we will be looking at large, complicated organic molecules and we will want to refer to a small portion of that molecule by name without referring to the whole molecule. To take a simple example, let's look at the branched isomer of butane:



We can regard this molecule as being a chain propane molecule with a CH_3 group being substituted on the middle carbon atom and providing a branch point. Note that this CH_3 group is almost but not quite a methane molecule. There is one less H atom so that the CH_3 group can be bonded by its fourth bond to the propane chain. We call this CH_3 group a **methyl** group.

Similarly in the molecule:



We have a $-CH_2CH_3$ group being branching off of the middle C atom of a pentane molecule. Again the $-CH_2CH_3$ group is almost an ethane molecule except that one hydrogen has been removed so that the bond can be used to attach the group to the main chain. The $-CH_2CH_3$ group is called an **ethyl group.**

These are names for alkyl groups for any given number of carbons, but we will be concerned only with the names for chains ranging from 1-10 carbon atoms.

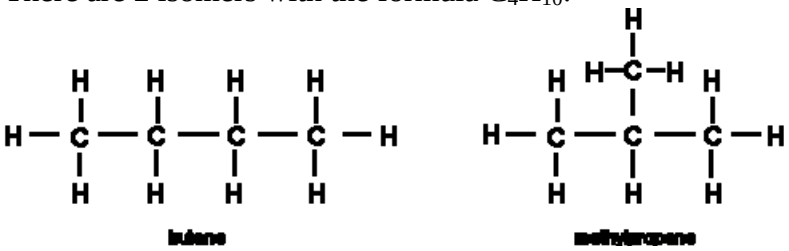
Number of C Atoms	Name
1	methyl
2	ethyl
3	propyl
4	butyl
5	pentyl

6	hexyl
7	heptyl
8	octyl
9	nonyl
10	decyl

The first four names (which are by far the most common) can be remembered by the mnemonic device:

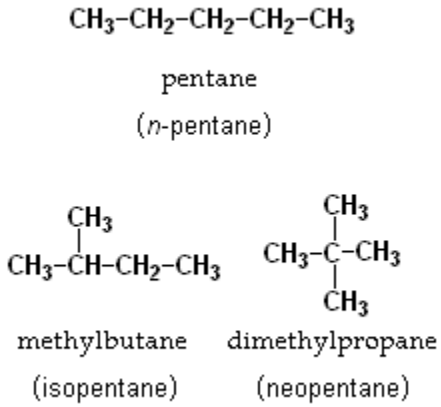
Methyl, ethyl
Propyl, butyl
After that,
It's all futile!

There are 2 isomers with the formula C_4H_{10}:



The unbranched chain isomer is called butane as indicated by the rules given above. The branched chain isomer was originally called isobutane, because it was an isomer of butane.

For the formula C_5H_{12} there are 3 isomers as shown below. The first molecule is the unbranched chain pentane; the second molecule has a methyl(-CH_3) branch off of a 4-C chain, and the third has 2 methyl(CH_3) groups coming off the middle C atom of the 3 carbon chain:



The first molecule is called pentane as before; the second isomer was called isopentane, and the third isomer was called neopentane because it was a new isomer (neo-is the Latin for new).

If we look at the table below however, we see that naming these isomers by simply putting prefixes in front of the name of the straight chain isomer will not be a very easy task for organic molecules containing a large number of C atoms. We will simply run out of names.

Chemical Formula	Number of Isomers
C_6H_{14}	5
C_7H_{16}	9
$C_{10}H_{22}$	75
$C_{15}H_{32}$	4347
$C_{40}H_{82}$	62,500,000,000,000

Clearly a more systematic way of naming molecule is necessary and organic chemists have developed such a system, called IUPAC nomenclature (International Union of Pure and Applied Chemistry). We will present the rules necessary to name alkanes in this unit, and will present additional rules for naming other functional groups in subsequent units. Although systematic names are used by professional chemists, it should be noted that most drug and food molecules are referred to by common non-systematic names. These names must simply be memorized.

Rules of Systematic Nomenclature

1. Name the longest (straight) unbranched carbon chain in the structure.

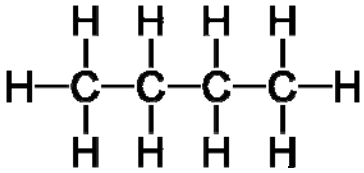
2. Preceding the name of the longest chain, write down in alphabetical order the names of each of the alkyl groups which are attached to the main chain.

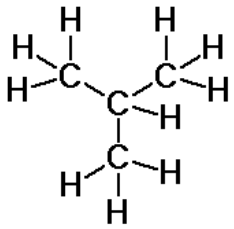
3. If there are several groups of the same kind, list the group only once, using appropriate prefix: di- for 2, tri- for 3, tetra- for 4, penta- for 5, hexa- for 6, hepta- for 7, octa- for 8 to indicate how many of the groups there are.

4. Assign a number, as a prefix, to each of the alkyl groups in the name to indicate the position of the group on the main chain. Start numbering from whichever end of the main chain results in the lowest sum of numbers.

.Examples: Draw and name

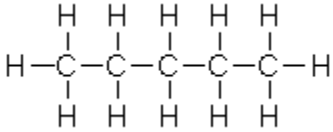
2 isomers of butane (C_4H_{10})



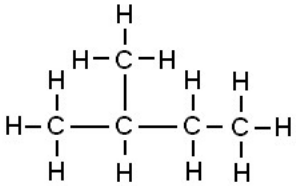


butane (as before) 2-methylpropane

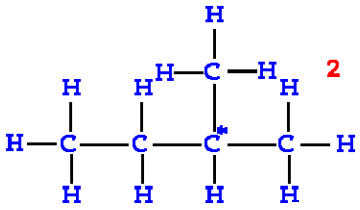
3 isomers with the formula (C_5H_{12})



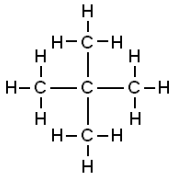
pentane (as before)



2-methylbutane
longest chain is 4 C's, so name compound as a derivative of butane with a methyl group hanging on 2nd C from the end



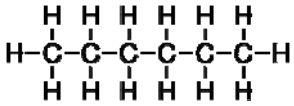
We might draw
as still another isomer and name it 3-methylbutane. Closer inspection shows that if we simply flip the molecule over from left to right we will have 2-methylbutane, which is the preferred name, since it has a smaller number.

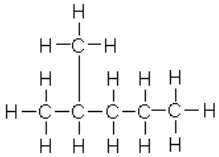


2,2-dimethylpropane
longest "straight" chain is 3C's so
name it propane; two methyl groups hanging off second C so we have 2,2-dimethylpropane

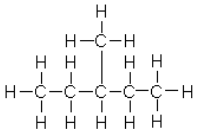
Note that IUPAC rules require that the number 2 be repeated to make it absolutely clearly that both methyl groups are on #2 C of the unbranched chain.

Draw 4 isomers with formula C_6H_{14}

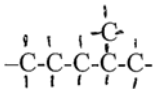
Solution: 1)  hexane

2)  2-methyl pentane. (We want to start numbering from left to right to keep the numbering as small as possible.

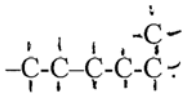
If we move the branch down one C on the main chain we have:



The name of this molecule is 3-methyl pentane and it does not matter from which end of the molecule we start the numbering.

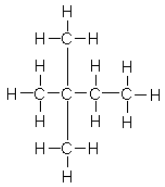
If we move the methyl group down another C on the main chain we have 

You might initially think this is a new isomer, 4-methylpentane, but closer inspection should make you realize this molecule is the same as 2-methylpentane, just flipped from left to right.

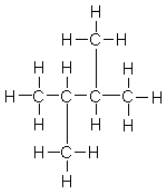
If we move the methyl branch 1 C further down the chain we have  .

Careful inspection of this conformation should reveal that it is NOT a branched isomer at all. It is just a different conformation of an unbranched 6 C hexane chain. It may be easier to visualize this if you take a pencil (or pen) and start from left to right. You can cover all 6 C atoms in one continuous stroke of the pencil.

4) There are however two more isomers of C_6H_{14} which have two methyl groups branching off a 4 C unbranched chain.

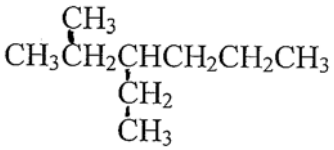


2,2 dimethylbutane



2,3 dimethylbutane

Additional naming practice:

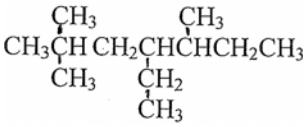


a)
The longest straight chain is 6 C's so name it hexane; add the branching chains in alphabetical order: ethyl and methyl. We still need to indicate where the ethyl and methyl groups are hooked on and that's where the numbers come in. Numbering from left to right we obtain:

3-ethyl-2-methylhexane Sum of numbers is 5

Numbering from right to left: 4-ethyl-5-methylhexane. The sum of the numbers is 9, so numbering from left to right is preferred.

Draw the line-bond notation for the above molecule.



b)Name:
Longest straight chain, ignoring branches, is 7 carbons.

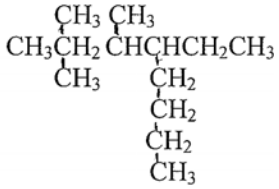
We have 3 methyl groups and one ethyl group branching off the main chain so our in front we have ethyl trimethyl

Now add the numbers, try starting from either end (then add the sum of the numbers).

Numbering from left to right we get 4-ethyl-2,2,5-trimethylheptane. Sum of #'s is 13

Numbering from the right to left we have 4-ethyl-3,6,6-trimethylheptane.Sum of #'s is 19
First answer is correct name because the sum of numbers is smaller.

c)Name



At first glance it might appear that the longest chain(reading straight across) has 6 C, but look again and notice there is a 4 C branch on C #4 (from the left). This "branch" is longer than the 2 C chain continuing horizontally. Since free rotation allows putting the chain in whichever direction we wish, the longest unbranched chain contains 8 C atoms

Numbering from left to right we have:
4-ethyl-2,2,3-trimethyloctane. Sum of numbers is 11
Number from right to left we have
5-ethyl-6,7,7 trimethyloctane. Sum of numbers is 25
First name is the correct one.