Alkane

Alkanes:

The first classification for organic molecules is the most simple, the alkane. The most simple alkane consists of only carbon and hydrogen atoms connected by single bonds. Alkanes are common and for the most part chemically uncreative, the chemical reaction combustion being the major exception. Alkanes can be found in many common substances; natural gas, gasoline, plastics…The chemical formula can be generalized as:

$$C_nH_{2n+2}$$

Where ***n*** represents the number of carbons and 2n+2 equals the number of hydrogen's.

Nomenclature:

Nomenclature is the scientific term for naming compounds. The governing body is "The International Union of Pure and Applied Chemistry", or IUPAC for short. The following statement is from their web site:

"The International Union of Pure and Applied Chemistry (IUPAC) serves to advance the worldwide aspects of the chemical sciences and to contribute to the application of chemistry in the service of Mankind. As a scientific, international, non-governmental and objective body, IUPAC can address many global issues involving the chemical sciences."

IUPAC was formed in 1919 by chemists from industry and academia. One of there main functions is to objectively create rules for naming compounds in the most simplified manner possible. This is equivalent to creating a new language, just like English grammar, there are rules .Even with the advent and acceptance of the IUPAC system some common names still persist, when discussing a substance the IUPAC name should be used but the common name will be accepted by most chemical organizations.

Alkane Nomenclature:

Naming of organic structures, unlike biological classification, follows a rigid set of rules. The International Union of Pure and Applied Chemistry, abbreviated IUPAC, came up with a set of rules that follows the same standards worldwide, and is accepted among all chemists. However,

common names of compounds, or names that have historical roots, are still used today for many compounds.
The suffix for the alkane family is –***ane***.

prefix – root – suffix

prefix – where the substitutions are located
root – how many carbons are in the molecules longest chain
suffix – family – type of functional group (alkane, alkene, alcohol, ester, etc...)

Root words are named for its number of carbons:

No. of carbons	***root***
1	meth-
2	eth-
3	prop-
4	but-
5	pent-
6	hex-
7	hept-
8	oct-
9	non-
10	dec-

Example:
an alkane with 3 carbons is named propane
prop – for the 3 carbons
ane – for the family alkane (meaning all single bonds)

Formula Types:

A variety of methods are used to describe a chemical compounds composition. Sometimes you will find a the chemical formula sufficient. Other times you need to see the structure drawn out, this is referred to as the structural formula. This is a larger drawing which will show the atoms are connected. Another is the condensed structural formula, this shows the connections in around about manner. Lastly, a more lazy form is the line structure. This simplified drawing assumes you know that carbon atoms make 4 bonds and that if you do not see a bond drawn assume a hydrogen is

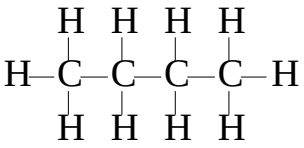
occupying the undesignated bond. Also all ends and turns in the line signify carbon atoms.

Examples:

Chemical Formula:

C_4H_{10}

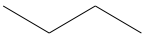
Structural Formula:



Condensed Structural Formula:

$CH_3CH_2CH_2CH_3$

Line Structure:



Rules:

1. Find the longest chain of carbons, and use this number as the base/root/parent name .

2. Number the chain with the end nearest the first subsistent carbon #1.

3. Give the location of the alkyl subsistent by the number of the main-chain carbon that it is attached to.

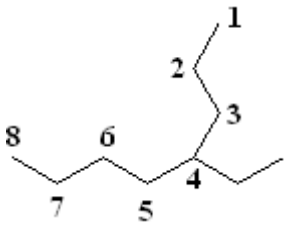
Put the Constituents in alphabetical order (i.e. ethyl before methyl)

4. Substitution Syntax:

a.between numbers and words add a dash

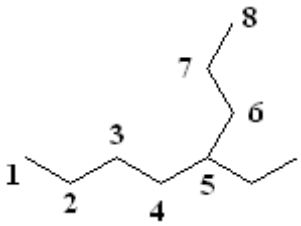
b.between numbers add commas

Examples:



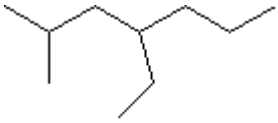
4-Ethyl-octane

Correct

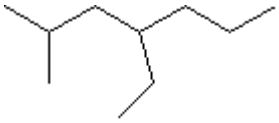


5-Ethyl-octane

Incorrect



4-Ethyl-2-methylheptane
Correct



4-Ethyl-6-methylheptan
Incorrect

Exercises

1. Name the following hydrocarbons and write their formulas.



Draw a line drawing of a “straight-chain” alkane with 12 carbon.

2. atoms. Use the general formula to determine the number of hydrogen atoms that it has.

Side Chain Specific Rules:

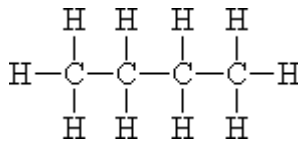
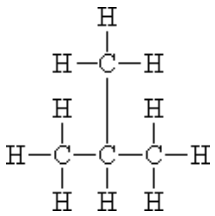
4-propyloctane	4-isoproplyoctane
$CH_3CH_2CH_2CH_2CH(CH_2CH_2CH_3)CH_2CH_2CH_3$	$CH_3CH_2CH_2CH_2CH(CH_2CH_2CH_3)CH_2CH_2CH_3$

Isomers:

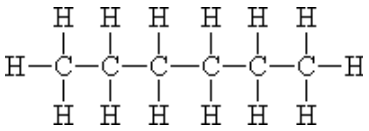
Isomerization - same molecular formula, but different structure. Also creates different properties for the molecule. The number of possible isomers increases rapidly as the length of the chain increases. These molecules are isomers of the same chemical formula.

Examples:

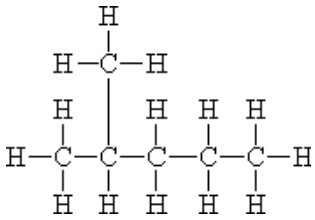
Each of the following molecules has a chemical formula of C_4H_{10} but they are different molecules having different properties.

Butane	2-methyl propane (isobutane)
	

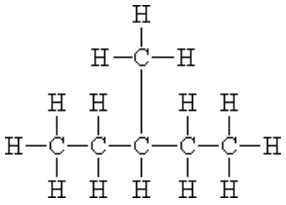
More Examples:



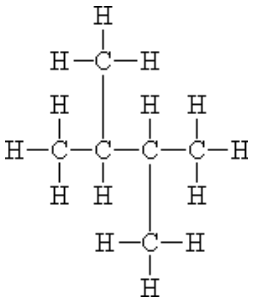
hexane



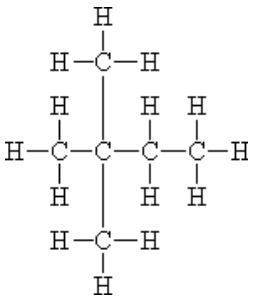
2-methyl pentane



3-methyl pentane



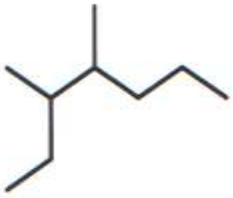
2,3-dimethyl butane

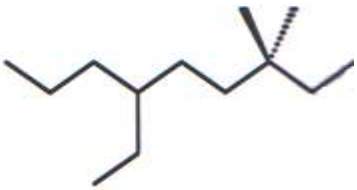


2,2-dimethyl butane
not
3,3-dimethyl butane

Exercises

3. Apply the rules and name the following alkanes.





4. Draw the structures for the following alkanes:

a. 4-methyldecane

b. 2, 3-dimethyl-4-propyloctane

c. 3-ethyl-4,4,5-triethylnonane

Cyclic Alkanes:

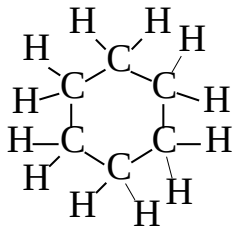
Alkanes can form compounds with themselves. By this I mean they commonly form rings. Shown below is cyclohexane. It is a hexane molecule that has come around back onto itself. The below you will find the chemical formula, structural formula and the line diagram.

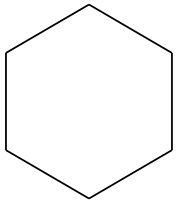
Nomenclature of Cycloalkanes general Formula: C_nH_{2n}

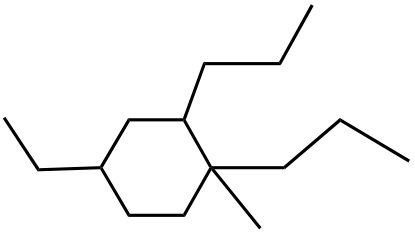
This is the same as for alkanes, although two extra rules apply.

Rule A: Decide whether the cyclic or acyclic portion contains more carbons. This determines the base name. (Alkyl substituted cycloalkane or cycloalkane substituted alkane).
Rule B: Carbons are numbered to give the lowest numbers for substituted carbons.

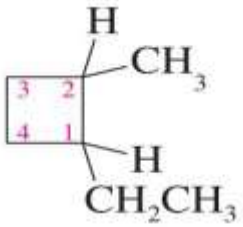
Examples:



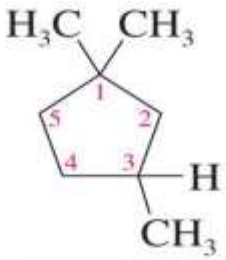




Numbering starts at the most substituted carbon, and goes around in order to give the lowest numbers.

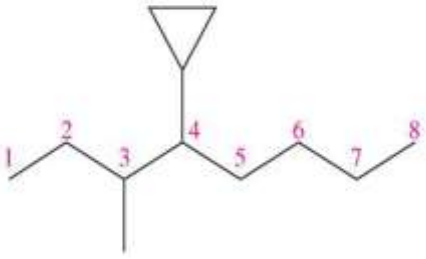


1-ethyl-2-methylcyclobutane

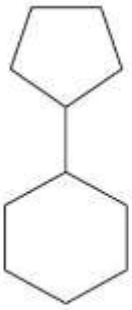


1,1,3-trimethylcyclopentane

When there are more acyclic than cyclic carbons, the cyclic part becomes a cycloalkyl substituent.



4-cyclopropyl-3-methyloctane



cyclopentylcyclohexane