

Alkanes

1 - Aliphatic Nomenclature

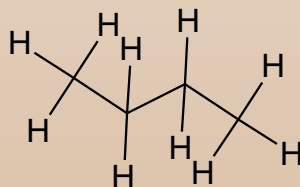
Dr. Sapna Gupta

Alkanes Review

- **Hydrocarbon:** A compound composed only of carbon and hydrogen.
- **Saturated hydrocarbon:** A hydrocarbon containing only single bonds.
- **Alkane:** A saturated hydrocarbon whose carbons are arranged in an open chain.
- **Aliphatic hydrocarbon:** Another name for an alkane.
- **Organic Structures** – review
 - *Molecular formula* - C_4H_{10}
 - *Condensed structure* - $CH_3CH_2CH_2CH_3$

- *Structural formula*

- Expanded structure



- Line structure



Naming Organic Compounds

Organic compounds are named according to IUPAC* rules which is quite systematic. Two important components of naming include the number of carbons and functional groups.

- The table on the right gives the prefixes used for carbons 1-10 (*most common for us*).
- Organic nomenclature follows the rules of a prefix to indicate the number of carbons (the **alk**) and the suffix to indicate the functional group. Numbers are used to indicate where those functional groups are located.

For example:

2 carbon **alkane** – **ethane**

2 carbon **alkene** – **ethene**

2 carbon alcohol – **ethanol**

As we go through organic chemistry, we will learn how to name each functional group systematically.

**International Union of Pure and Applied Chemistry*

No. of Carbons	Formula	Name
1	C	Meth
2	C ₂	Eth
3	C ₃	Prop
4	C ₄	But
5	C ₅	Pent
6	C ₆	Hex
7	C ₇	Hept
8	C ₈	Oct
9	C ₉	Non
10	C ₁₀	Dec

Naming Straight Chain Alkanes

Here are the names for alkanes from carbon 1-20, with some missing in the middle. We will focus more on naming compounds of carbons 1-10.

Follow the steps shown in the next slides to learn how to name alkanes.

No. of Carbons	Formula	Name		No. of Carbons	Formula	Prefix
1	CH ₄	Methane		8	C ₈ H ₁₈	Octane
2	C ₂ H ₆	Ethane		9	C ₉ H ₂₀	Nonane
3	C ₃ H ₈	Propane		10	C ₁₀ H ₂₂	Decane
4	C ₄ H ₁₀	Butane		11	C ₁₁ H ₂₄	Undecane
5	C ₅ H ₁₂	Pentane		12	C ₁₂ H ₂₆	Dodecane
6	C ₆ H ₁₄	Hexane		13	C ₁₃ H ₂₈	Tridecane
7	C ₇ H ₁₆	Heptane		20	C ₂₀ H ₄₂	Icosane

Some General Nomenclature Rules

prefix-infix-suffix

- **Prefix:** Tells the number of carbon atoms in the parent chain.
- **Infix :** Tells the nature of the carbon-carbon bonds in the parent chain.
- **Suffix :** Tells the class of the compound. (This can also be infix depending on the functional group).

No. of Carbons	Prefix
1	Meth
2	Eth
3	Prop
4	But
5	Pent
6	Hex
7	Hept
8	Oct
9	Non
10	Dec

Infix	Nature of C-C bond
-an-	Single bonds
-en-	One or more double bonds
-yn-	One or more triple bonds

Suffix	Functional Group
-e	Hydrocarbon
-ol	Alcohol
-al	Aldehyde
-amine	Amine
-one	Ketone
-oic acid	Carboxylic acid

Some General Nomenclature - Examples

prefix-infix-suffix

prop-**en**-e = propene



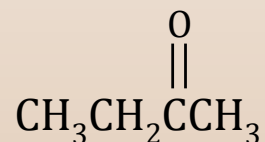
eth-**yn**-e = ethyne



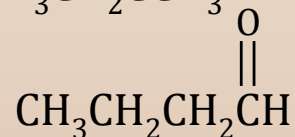
eth-**an**-ol = ethanol



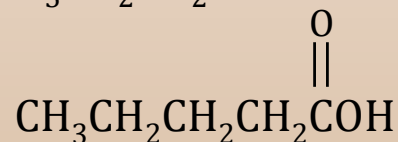
but-**an**-one = butanone



but-**an**-al = butanal



pent-**an**-oic acid = pentanoic acid



eth-**an**-amine = ethanamine



Nomenclature Alkanes - Rules

1. Find the longest continuous carbon chain.
2. Number the carbons, starting closest to the first branch.
3. Numbering starts from the end of the chain which is closest to the group named in the suffix.
4. Name the groups attached to the chain, using the carbon number as the locator.
5. Alphabetize substituents.
6. Use di-, tri-, etc., for multiples of same substituent. (Don't use these for alphabetizing substituents).
7. An IUPAC name may have up to 4 features: locants, prefixes, parent compound and suffixes.

See the next slide for a pictorial and other key things to writing a name.

Nomenclature Alkanes - Rules

Some other things to remember:

1. Use hyphens “-” between number and letter, e.g. 3-methylhexane.
2. Use comma “,” between two numbers, e.g. 2,3-dimethylhexane.
3. There is no space between substituent and parent name in case there is no locant, e.g. 3-methylhexane.
4. As we learn more nomenclature, we will add more rules.

Locant - Prefix - Parent - Suffix

Where the substituent and functional groups are located

What are the substituent

The longest carbon chain

The highest priority functional group



4-methyl-1-hexanol

locant

prefix

locant

parent

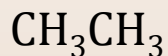
suffix

Nomenclature of Alkanes – Getting Started

The first three alkanes can be named just by counting the number of carbons.



methane



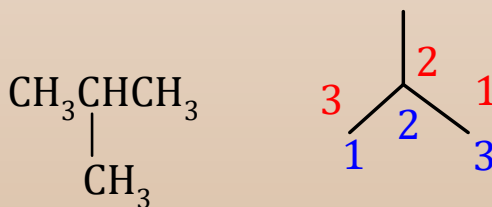
ethane



propane

The fourth alkane $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$ is butane. A constitutional isomer of butane can be drawn as $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_3$. Even though it has four carbons, it cannot be called butane as that name is only for a straight chain structure.

Following the rules of nomenclature, find the longest chain. It is best to draw the carbon chain or line structure at this point to help see the structure clearly.

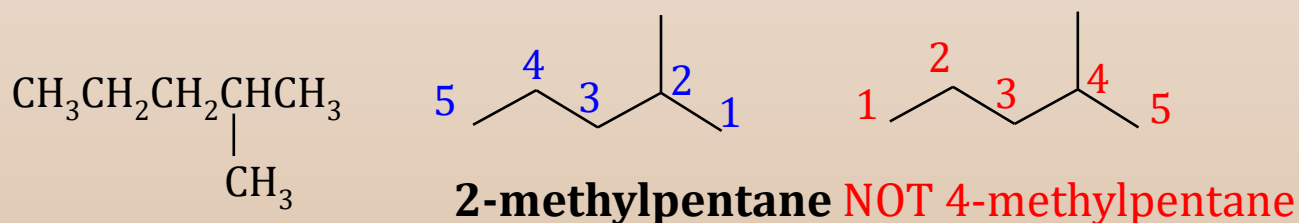


The longest chain is 3 carbon so base name is propane. On the 2nd carbon is a methyl group – 2-methyl. Since this is a small chain, numbering from either side (*red or blue numbers*) will give the methyl group at carbon 2. The name is therefore: 2-methylpropane.

Nomenclature Alkanes-2

Here is another example with longer chain and one substituent.

- The parent chain is the longest chain of carbon atoms. In the example below it is pentane.
- The substituent is named and assigned a locant number. Use a hyphen to connect the number to the name. In the example below the substituent* is methyl. The locant can be 2 or 4. but the rule is to always give the lower number to the substituent, so the location will be **2-**.



*A substituent is called as such because that group is substituting a hydrogen on that carbon. A substituent can be an alkyl group or functional group.

Alkyl Groups

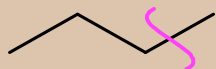
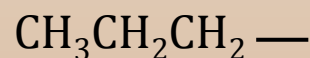
Alkyl groups are alkanes minus 1H on them. The alk in the name indicates the number of carbons and yl ending tells you that it is a substituent.

CH_4 is methane and CH_3 is methyl. Note that CH_3 cannot exist on its own, because carbon has only 3 bonds, which is why there must be a connection point on the carbon, which in case of CH_3 is on the only carbon there is.

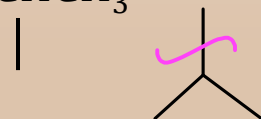


For CH_3CH_3 ethane, the alkyl group is ethyl, CH_3CH_2- or $-\text{CH}_2\text{CH}_3$. Whichever side has the one less hydrogen is where the bond will be.

$\text{CH}_3\text{CH}_2\text{CH}_3$ is propane, $\text{CH}_3\text{CH}_2\text{CH}_2-$ is propyl, and the bond is on the carbon with less hydrogens. However, in propyl group there can be two connection points, one on the 1st carbon and 2nd on the 2nd carbon as shown below. Both are not the same as seen in the line structure, hence their names are also different, as given below the structures.



Propyl



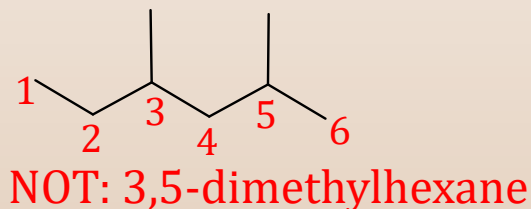
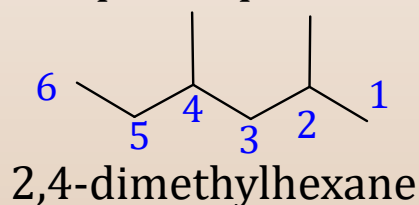
isopropyl

(Note: The pink curved line is drawn to show where the connection is.)

Nomenclature Alkanes-3

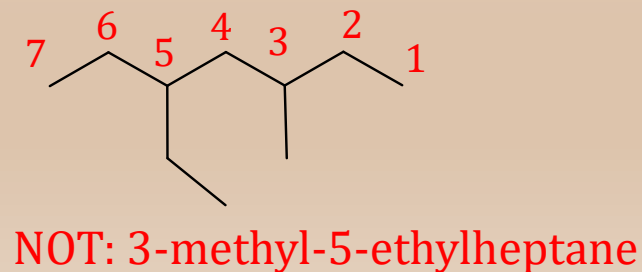
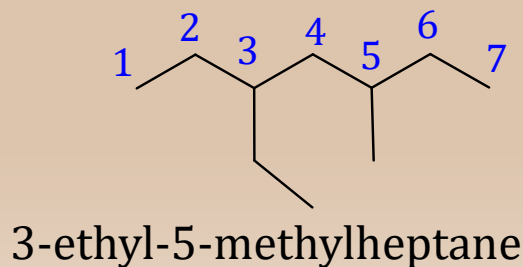
If there are two or more identical substituents, number the chain from the end that gives the lower number to the substituent encountered first.

- Indicate the number of times the substituent appears by a prefix di-, tri-, tetra-, etc.
- Use commas to separate position numbers.



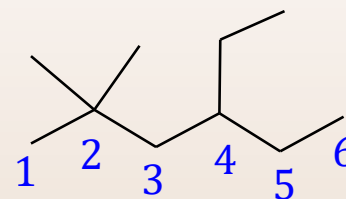
If there are two or more different substituents,

- list them in alphabetical order.
- number from the end of the chain that gives the first substituent or where the first branching occurs.
- write the substituents in alphabetical order, NOT in chronological order.



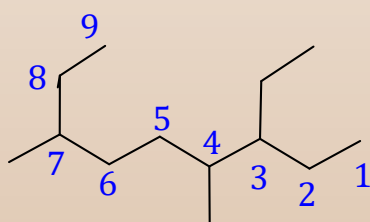
Nomenclature Alkanes-4

- The prefixes di-, tri-, tetra-, etc. are not included in alphabetization.
- Alphabetize the names of substituents first and then insert these prefixes.
- Here are more examples.



4-ethyl-2,2-dimethylhexane

NOT: 2,2-dimethyl-4-ethylhexane

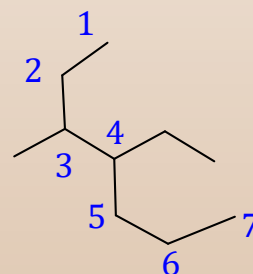
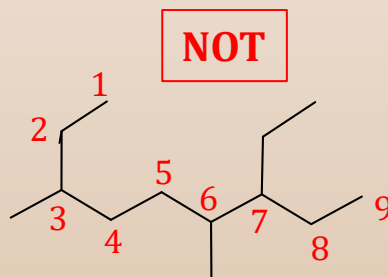


Substituents: On C3 – ethyl
C4 – methyl
C7 – methyl

Longest chain 9C - nonane

Name: 3-ethyl-4,7-dimethylnonane

NOT: 7-diethyl-3,6-dimethylnonane

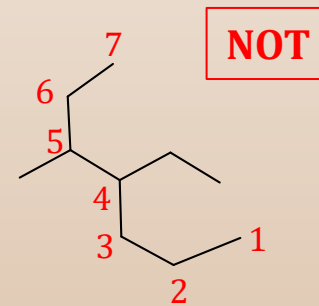


Substituents: On C3 – methyl
C4 – ethyl

Longest chain 7C - hexane

Name: 4-ethyl-3-methylheptane

NOT: 4-ethyl-5-methylheptane

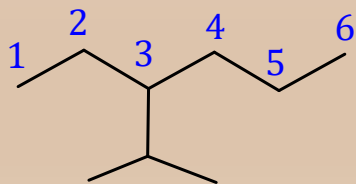


Alkyl Groups – A Detailed Look

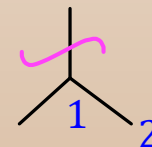
Let's continue to look at isopropyl group and see a different way to name alkyl groups.

Isopropyl group is non IUPAC name, or general name, however, IUPAC has approved of this name to be used as official name. So what is the official name of isopropyl? We name it as an alkane by numbering the longest chain, starting from the bond and then numbering any substituent from the closest to the branching.

Looking at the group now, the carbon chain is 2 carbon long, and there is a methyl group on the 1st carbon. The IUPAC name is (1-methylethyl). The entire name is written in parenthesis since it is a substituent. The locant of this group is placed before the group, as usual. The compound below can be named as 3-isopropylhexane OR 3-(1-methylethyl)hexane.



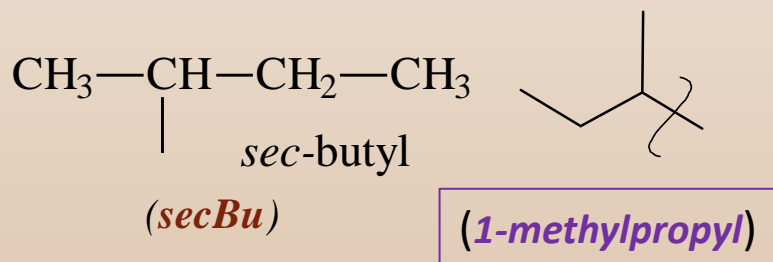
One last note on isopropyl, in isopropyl the “i” is used alphabetically. If there is a methyl and isopropyl, isopropyl precedes methyl in naming.



More on Alkyl Groups

Most of the alkyl groups are given on the next slide. I have given all possible structures and names for that alkyl group.

For the example below on a butyl isomer, see below where the carbon chain structure is given followed by the line structure. Sec-butyl is the name of the group, secBu is the shorthand and (1-methylpropyl) is the IUPAC name.



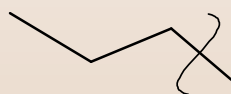
Remember that in isopropyl the “i” is used alphabetically. The same is not true for isobutyl. In isobutyl, it is the “b” that is used for alphabetical assignment.

Alkyl Groups (substituents)

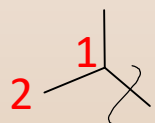
CH_3 - methyl (*Me*)

CH_3CH_2 - ethyl (*Et*)

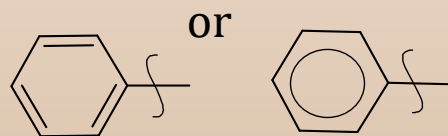
$\text{CH}_3\text{CH}_2\text{CH}_2$ - propyl (*Pr*)



CH_3 -CH- CH_3
|
isopropyl
(*iPr*)



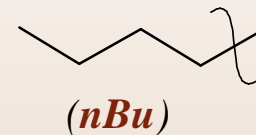
(1-methylethyl)



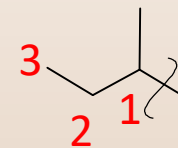
C_6H_5 — or Ph —

Phenyl group (Benzene connected on one carbon)

$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2$ -
n-butyl



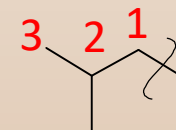
CH_3 -CH- CH_2 - CH_3
|
sec-butyl



(*secBu*)

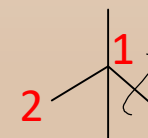
(1-methylpropyl)

CH_3 -CH- CH_2 -
|
 CH_3
isobutyl
(*iBu*)



(2-methylpropyl)

H_3C -C- CH_3
|
 CH_3
tert-butyl
(*tBu*)

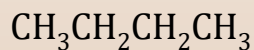


(2,2-dimethylethyl)

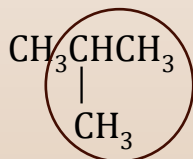
Alkane Nomenclature – General Names

Some common names of alkanes with four carbons are butanes, those with five carbons are pentanes, etc.

- **iso-** indicates the chain terminates in $-\text{CH}(\text{CH}_3)_2$; **neo-** that it terminates in $-\text{C}(\text{CH}_3)_3$.



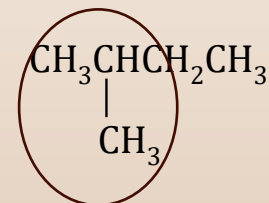
Butane



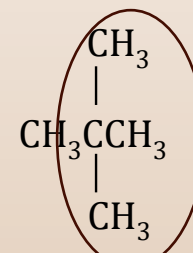
Isobutane



Pentane



Isopentane



Neopentane

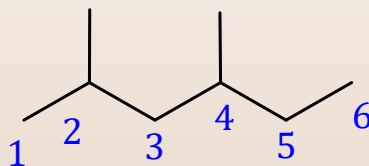
These names are common names and are used more in the lab than in lecture.

Solved Problem: Naming and Writing Structures

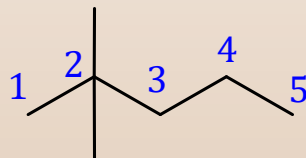
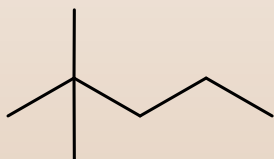
Write the names or draw the structures of the compounds given below.

ANSWERS

a) 2,4-dimethylhexane

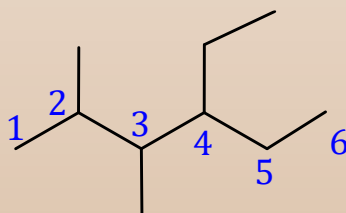
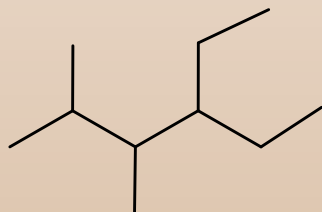


b)



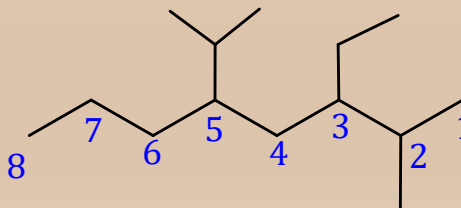
2,2-dimethylpentane

c)



4-ethyl-2,3-dimethylhexane

d) 3-ethyl-5-isopropyl-2-methyloctane



Solved Problem: Naming and Writing Structures

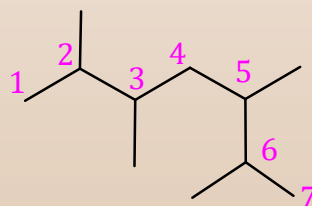
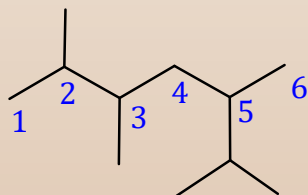
What is wrong with the names of the structures given below. Write the correct name.

- a) 5-isopropyl-2,3-dimethylhexane
- b) 5-isopropyl-2,3-diethylheptane

To answer this question you should draw the structure of the name given and then check the name for correctness.

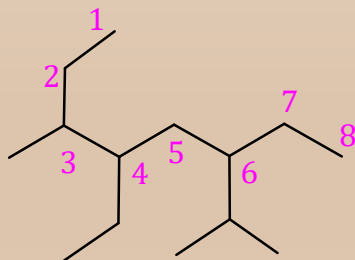
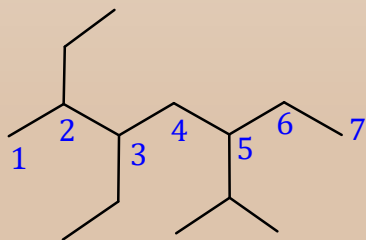
ANSWERS

- a) 5-isopropyl-2,3-dimethylhexane



The longest chain is heptane.
Correct name is:
2,3,5,6-tetramethylheptane

- b) 5-isopropyl-2,3-diethylheptane



The substituents are not in alphabetical order, and on drawing the structure the longest chain is octane. Correct name is: 4-ethyl-6-isopropyl-3-methyloctane
OR
3,5-diethyl-2,6-dimethyloctane
(renumber the structure and see it yourself! This name is correct but preferred is the top one because of fewer substituents)

Key Words/Concepts

- Identifying longest chain
- Naming all substituents
- Naming straight chain alkanes
- Fundamentals of nomenclature