

Alkane - 1 - Aliphatic Nomenclature

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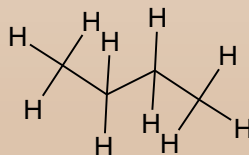
Structure

- 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 Straight Chain Alkanes

# of C	prefix
1	Meth
2	Eth
3	Prop
4	But
5	Pent
6	Hex
7	Hept
8	Oct
9	Non
10	Deca

Table 3.3 Names of Straight-Chain Alkanes

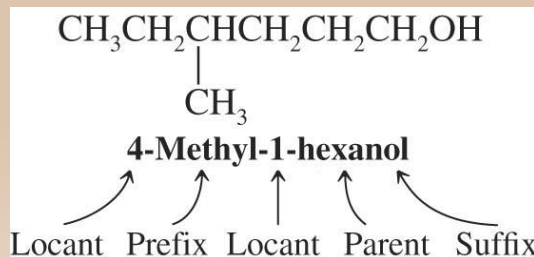
Number of carbons (<i>n</i>)	Name	Formula (C_nH_{2n+2})	Number of carbons (<i>n</i>)	Name	Formula (C_nH_{2n+2})
1	Methane	CH ₄	9	Nonane	C ₉ H ₂₀
2	Ethane	C ₂ H ₆	10	Decane	C ₁₀ H ₂₂
3	Propane	C ₃ H ₈	11	Undecane	C ₁₁ H ₂₄
4	Butane	C ₄ H ₁₀	12	Dodecane	C ₁₂ H ₂₆
5	Pentane	C ₅ H ₁₂	13	Tridecane	C ₁₃ H ₂₈
6	Hexane	C ₆ H ₁₄	20	Icosane	C ₂₀ H ₄₂
7	Heptane	C ₇ H ₁₆	30	Triacontane	C ₃₀ H ₆₂
8	Octane	C ₈ H ₁₈			

Nomenclature Alkanes-1

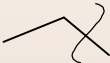
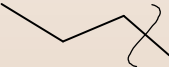
- Find the longest continuous carbon chain.
- Number the carbons, starting closest to the first branch.
- Name the groups attached to the chain, using the carbon number as the locator.
- Alphabetize substituents.
- Use di-, tri-, etc., for multiples of same substituent. (don't use these during alphabetizing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


Locant — **Prefix** — **Parent** — **Suffix**

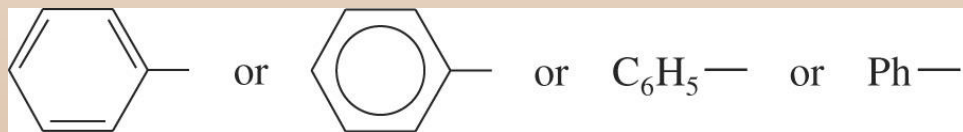
Where are the substituents and functional groups? What are the substituents? How many carbons? What is the primary functional group?



Alkyl Groups (substituents)

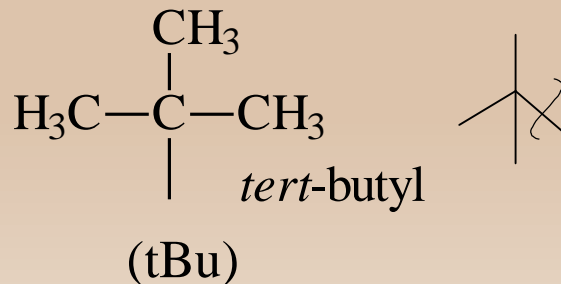
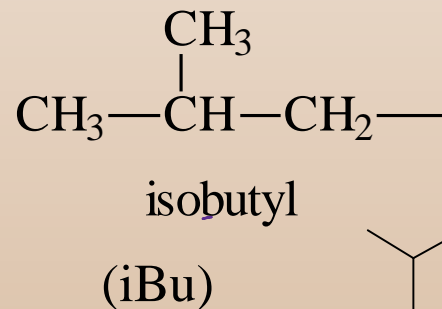
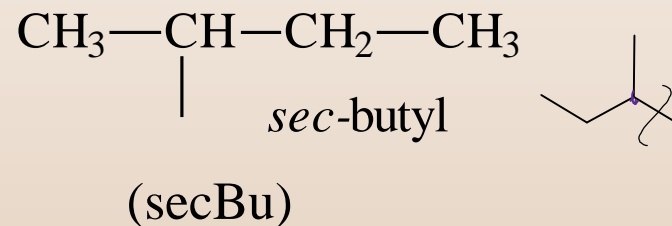
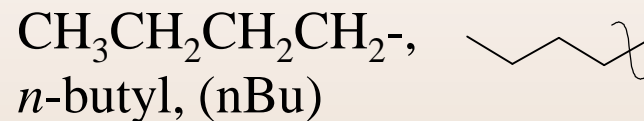
- CH_3- , methyl (Me)
- CH_3CH_2- , ethyl (Et) 
- $\text{CH}_3\text{CH}_2\text{CH}_2-$, *n*-propyl (nPr) 

- $\text{CH}_3-\text{CH}-\text{CH}_3$ (iPr)
|
isopropyl 



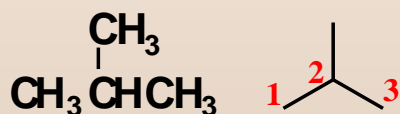
or $\phi-$ or Ar— (if ring substituents are present)

Phenyl group (Benzene
connected on one carbon)



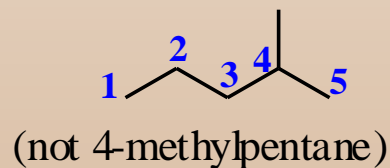
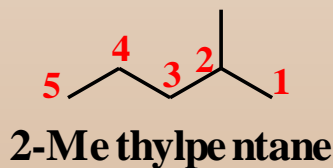
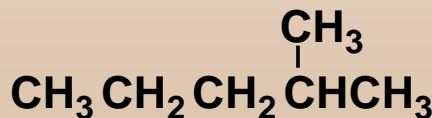
Nomenclature Alkanes-2

- The name of a saturated hydrocarbon with an unbranched chain consists of a prefix and suffix.
- The **parent chain** is the longest chain of carbon atoms.
- Each substituent is given a name and a number. Use a hyphen to connect the number to the name.



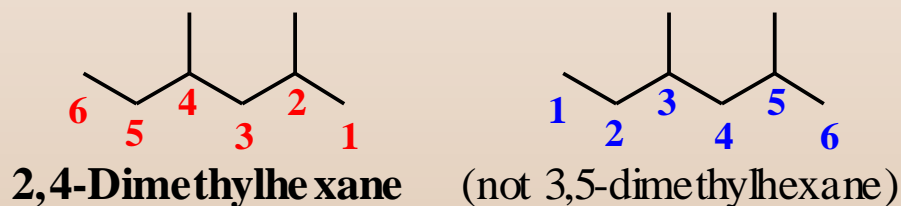
2-Methylpropane

- If there is one substituent, number the chain from the end that gives it the lower number.

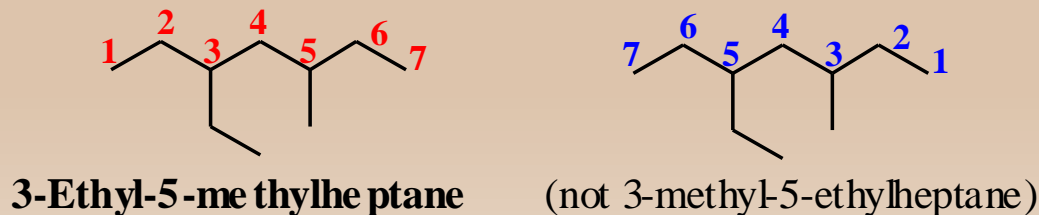


Nomenclature Alkanes-3

- 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

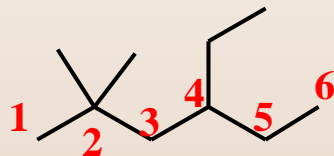


- If there are two or more different substituents,
- list them in alphabetical order.
- number from the end of the chain that gives the substituent encountered first the lower number



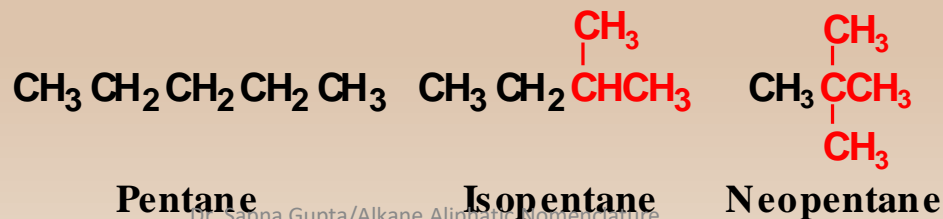
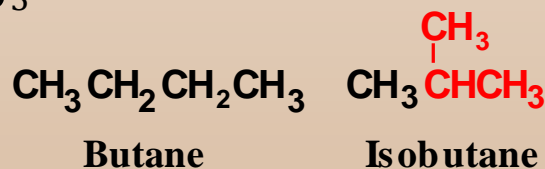
Nomenclature Alkanes-4

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



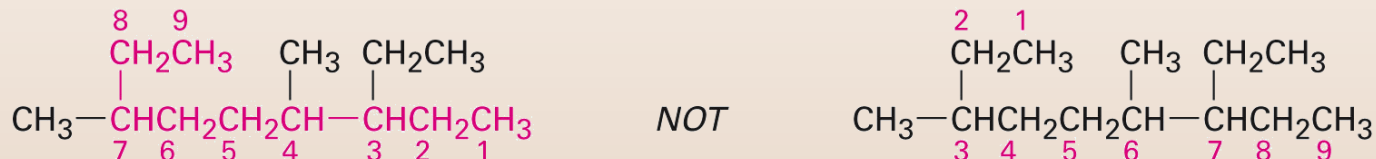
4-Ethyl-2,2-dimethylhexane
(not 2,2-dimethyl-4-ethylhexane)

- 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 $-\text{C}(\text{CH}_3)_3$.

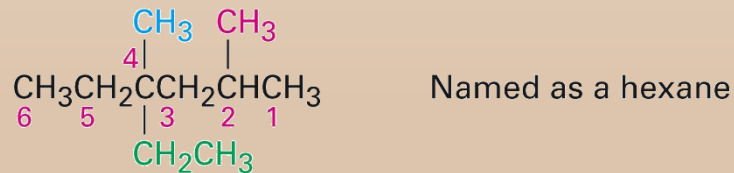
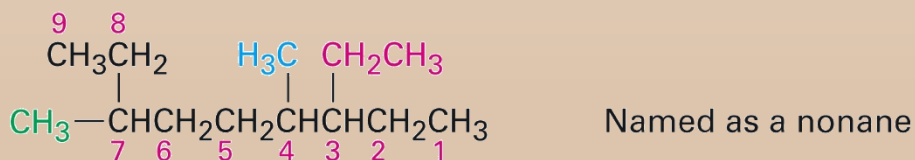


Nomenclature Alkanes-5

- Carbons in that main chain are numbered in sequence



- Substituents are identified and numbered

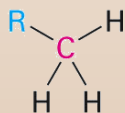


Substituents: On C3, CH_2CH_3 (3-ethyl)
 On C4, CH_3 (4-methyl)
 On C7, CH_3 (7-methyl)

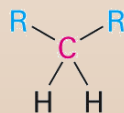
Substituents: On C2, CH_3 (2-methyl)
 On C4, CH_3 (4-methyl)
 On C4, CH_2CH_3 (4-ethyl)

Classification of Carbons and Hydrogens

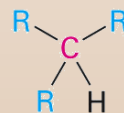
- Primary (1°) C: A carbon bonded to one other carbon.
 - 1° H: a hydrogen bonded to a 1° carbon
- Secondary (2°) C: A carbon bonded to two other carbons.
 - 2° H: a hydrogen bonded to a 2° carbon
- Tertiary (3°) C: A carbon bonded to three other carbons.
 - 3° H: a hydrogen bonded to a 3° carbon
- Quaternary (4°) C: A carbon bonded to four other carbons.



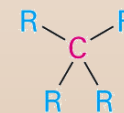
Primary carbon (1°)
is bonded to one
other carbon.



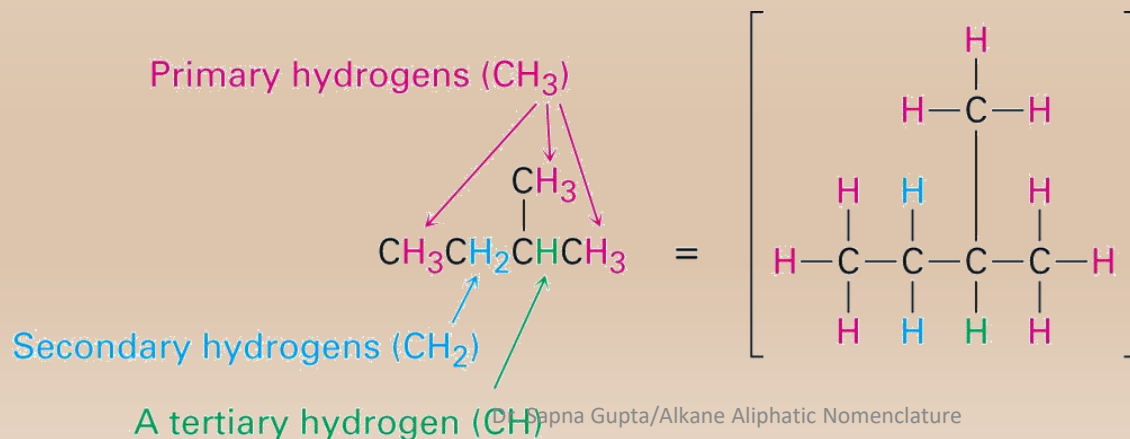
Secondary carbon (2°)
is bonded to two
other carbons.



Tertiary carbon (3°)
is bonded to three
other carbons.



Quaternary carbon (4°)
is bonded to four
other carbons.



Some General Nomenclature

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.

Infix	Nature of Carbon-Carbon Bonds in the Parent Chain
-an-	all single bonds
-en-	one or more double bonds
-yn-	one or more triple bonds

Suffix	Class
-e	hydrocarbon
-ol	alcohol
-al	aldehyde
-amine	amine
-one	ketone
-oic acid	carboxylic acid

Some General Nomenclature - Examples

prop-**en**-e = propene $\text{CH}_3\text{CH}=\text{CH}_2$

eth-**an**-ol = ethanol $\text{CH}_3\text{CH}_2\text{OH}$

but-**an**-one = butanone $\text{CH}_3\overset{\text{O}}{\parallel}\text{CCH}_2\text{CH}_3$

but-**an**-al = butanal $\text{CH}_3\text{CH}_2\text{CH}_2\overset{\text{O}}{\parallel}\text{CH}$

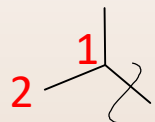
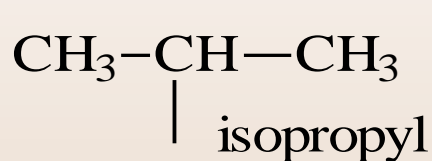
pent-**an**-oic acid = pentanoic acid $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\overset{\text{O}}{\parallel}\text{COH}$

cyclohex-**an**-ol = cyclohexanol 

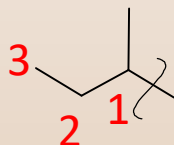
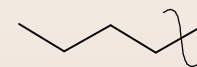
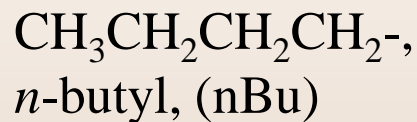
eth-**yn**-e = ethyne $\text{HC}\equiv\text{CH}$

eth-**an**-amine = ethanamine $\text{CH}_3\text{CH}_2\text{NH}_2$

One Last Thing on Alkyl Groups



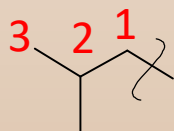
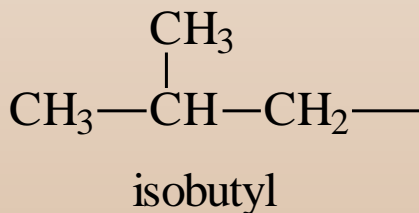
(1-methylethyl)



(1-methylpropyl)

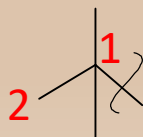
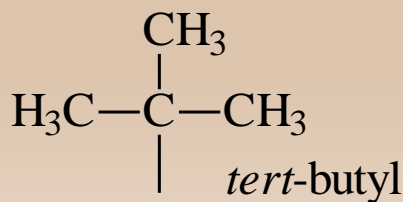
**No other name
as there is no
branching**

(secBu)



(2-methylpropyl)

(iBu)



(1,1-dimethylethyl)

(tBu)

Key Words/Concepts

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