Alkanes, Alkenes, Alkynes Cycloalkanes, Bicyclics, Alkyl Halides, Alcohols Nomenclature and Constitutional Isomers

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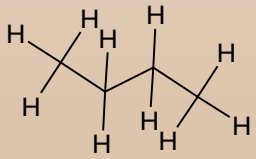
Structure

- 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.
- Alkanes are also called "Aliphatic" hydrocarbons.
- 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

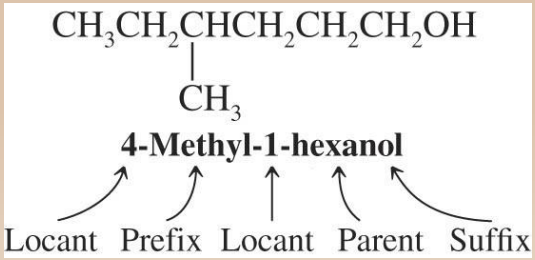
Number of carbons (n)	Name	Formula (C_nH_{2n+2})	Number of carbons (n)	Name	Formula (C_nH_{2n+2})
1	Methane	CH_4	9	Nonane	C_9H_{20}
2	Ethane	C_2H_6	10	Decane	$C_{10}H_{22}$
3	Propane	C_3H_8	11	Undecane	$C_{11}H_{24}$
4	Butane	C_4H_{10}	12	Dodecane	$C_{12}H_{26}$
5	Pentane	C_5H_{12}	13	Tridecane	$C_{13}H_{28}$
6	Hexane	C_6H_{14}	20	Icosane	$C_{20}H_{42}$
7	Heptane	C_7H_{16}	30	Triacontane	$C_{30}H_{62}$
8	Octane	C_8H_{18}			

Nomenclature Alkanes-1

1. Find the longest continuous carbon chain.
2. Number the carbons, starting closest to the first branch.
3. Numbering generally 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 during alphabetizing substituents)
7. An IUPAC name may have up to 4 features: locants, prefixes, parent compound and suffixes

Locant — Prefix — Parent — Suffix

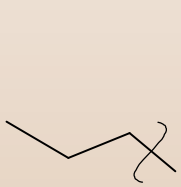
Where are the substituents and functional groups?	What are the substituents?	How many carbons?	What is the primary functional group?



Alkyl Groups (substituents)

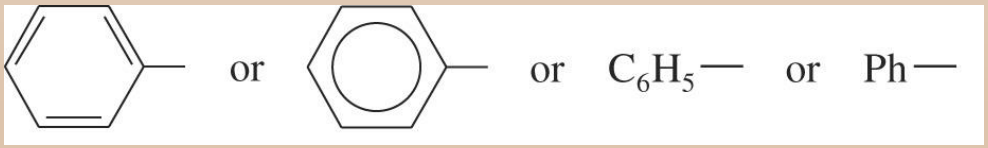
Alkyl groups are [alkane-1H]. The –yl ending on any group indicates that it is connected to a larger compound. Common substituents are up to 4C except for phenyl.

- CH_3-, methyl (Me)
- CH_3CH_2-, ethyl (Et)
- $CH_3CH_2CH_2$-, *n*-propyl (nPr)



- $CH_3-CH(-CH_3)$ (iPr)

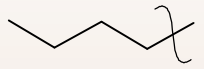
isopropy



or ϕ— or Ar— (if ring substituents are present)

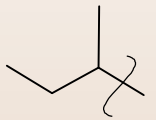
Phenyl group (Benzene connected on one carbon)

$CH_3CH_2CH_2CH_2$-,
n-butyl, (nBu)



$CH_3—CH(-CH_3)—CH_2—CH_3$

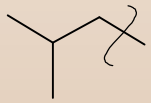
sec-butyl



(secBu)

$CH_3—CH(-CH_3)—CH_2—$

isobutyl



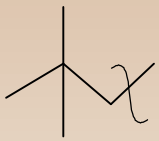
(iBu)

$H_3C—C(-CH_3)(-CH_3)—CH_3$

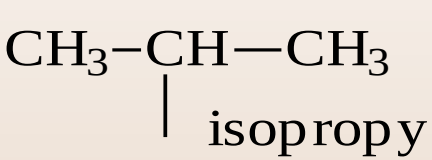
tert-butyl

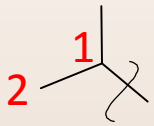
(tBu)

neopentyl



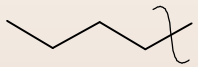
One More Thing on Alkyl Groups



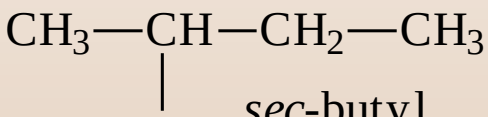


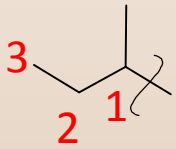
(1-methylethyl)

$CH_3CH_2CH_2CH_2$-,
n-butyl, (nBu)



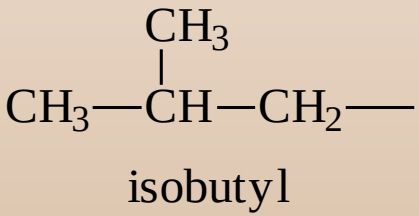
No other name as there is no branching

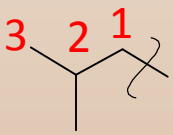




(1-methylpropyl)

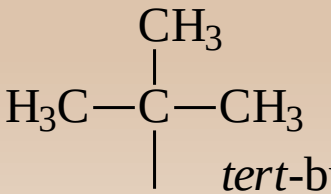
(secBu)

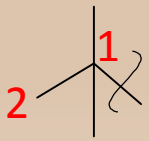




(2-methylpropyl)

(iBu)



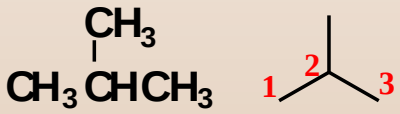


(1,1-dimethylethyl)

(tBu)

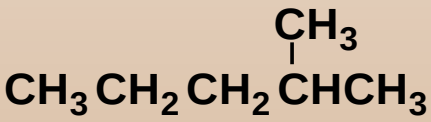
Nomenclature Alkanes-2

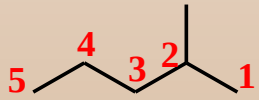
- The name of a saturated hydrocarbon with an unbranched chain consists of a prefix and suffix.
- The parent chain is the longest chain of carbon atoms.
- Each substituent is given a name and a number. Use a hyphen to connect the number to the name.



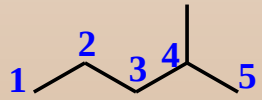
2-Methylpropane

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





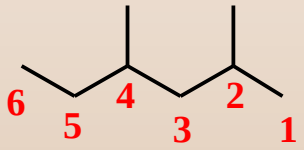
2-Methylpentane

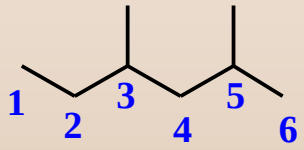


(not 4-methylpentane)

Nomenclature Alkanes-3

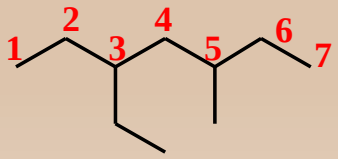
- If there are two or more identical substituents, number the chain from the end that gives the lower number to the substituent encountered first.
  - Indicate the number of times the substituent appears by a prefix di-, tri-, tetra-, etc.
  - Use commas to separate position numbers

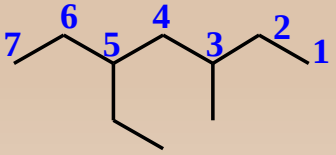




2,4-Dimethylhexane (not 3,5-dimethylhexane)

- 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

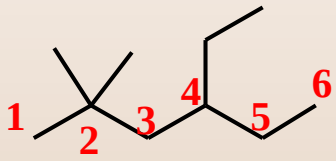




3-Ethyl-5-methylheptane (not 3-methyl-5-ethylheptane)

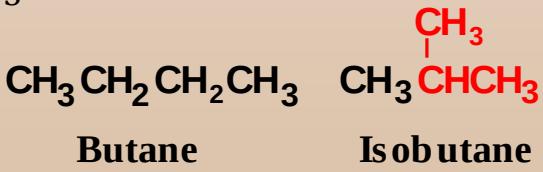
Nomenclature Alkanes-4

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

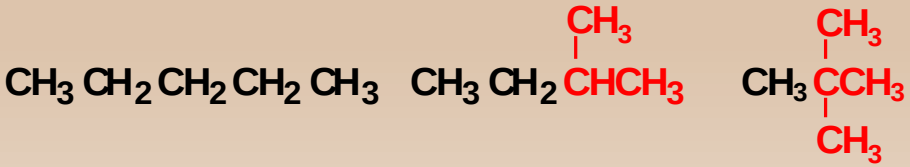


4-Ethyl-2,2-dimethylhexane
(not 2,2-dimethyl-4-ethylhexane)

- Some common names of alkanes with four carbons are butanes, those with five carbons are pentanes, etc.
- iso- indicates the chain terminates in -$CH(CH_3)_2$; neo- that it terminates in -$C(CH_3)_3$.



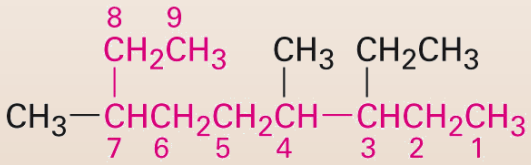
Butane **Isobutane**



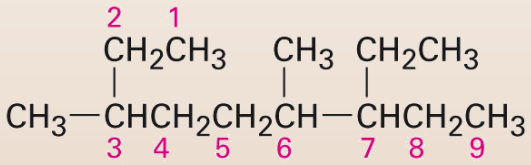
Pentane **Isopentane** **Neopentane**

Nomenclature Alkanes-5

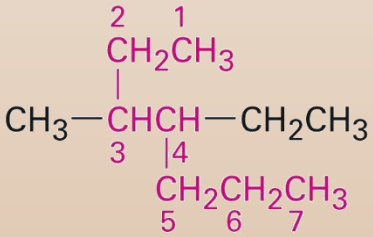
- Carbons in that main chain are numbered in sequence



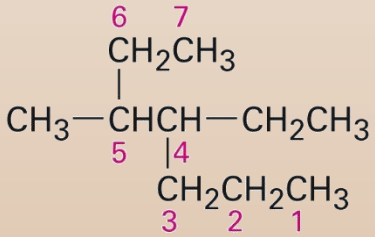
NOT

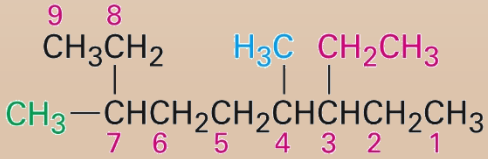


- Substituents are identified and numbered



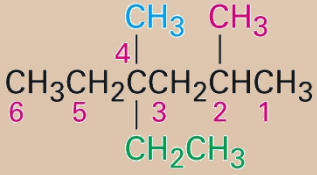
NOT





Named as a nonane

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

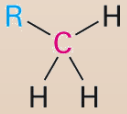


Named as a hexane

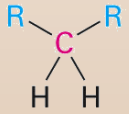
Substituents: On C2, CH_3 (2-methyl)
On C4, CH_3 (4-methyl)
On C4, CH_2CH_3 (4-ethyl)

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.



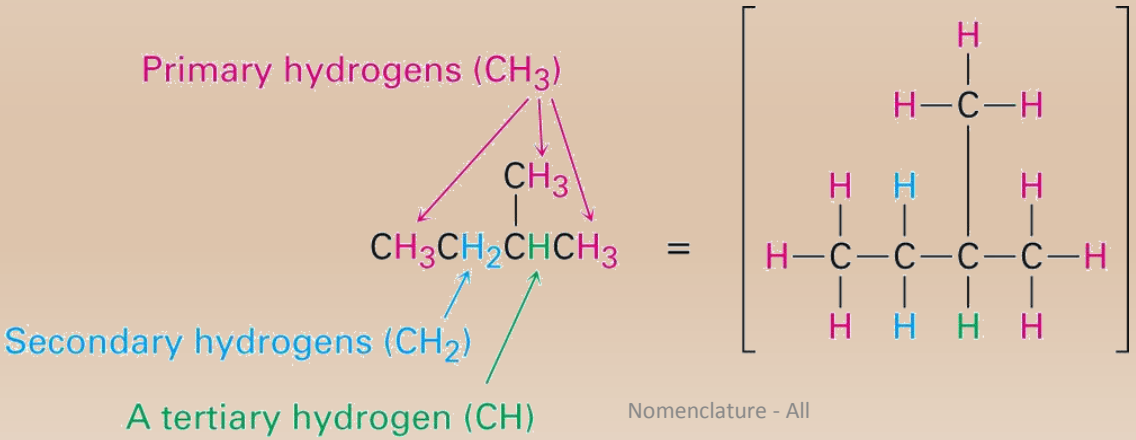
Primary **carbon (1°) is bonded to one other carbon.**



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

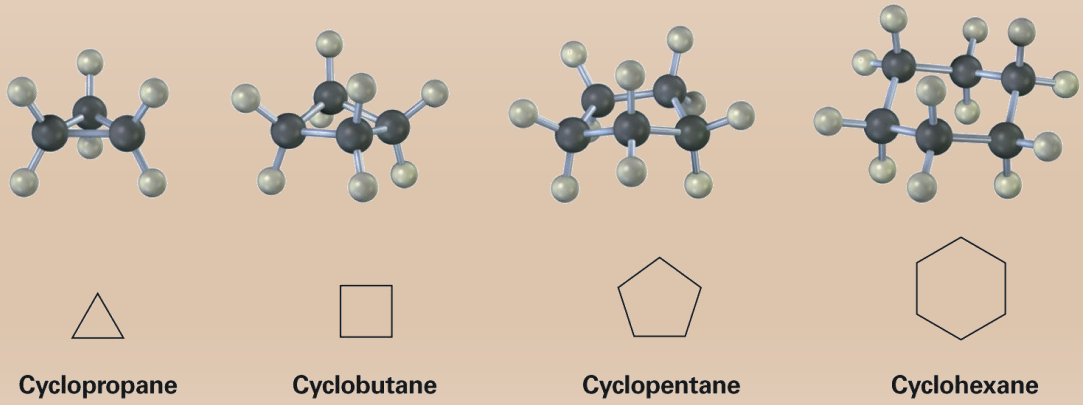
Tertiary **carbon (3°) is bonded to three other carbons.**

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

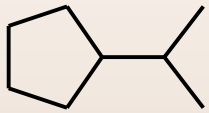


Cycloalkanes – Nomenclature

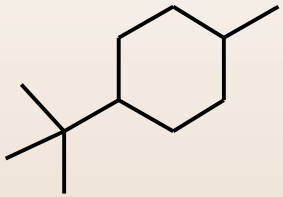
- Rings of carbon atoms (-CH_2- groups)
- Formula: C_nH_{2n}
- Cycloalkane name will usually be the base compound
- Number carbons in ring if >1 substituent
- First in alphabet gets lowest number if more than one substituent
- In case where a long chain is attached to cycloalkane then give the name of the chain with cyclic alkane as cycloalkyl group.



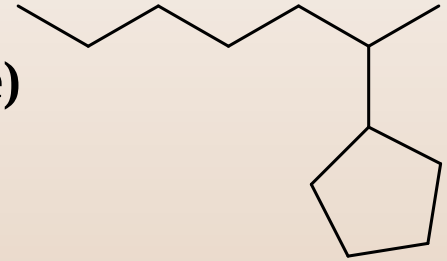
Naming Cycloalkanes

(a) 

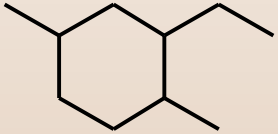
Isopropyl cyclopentane

(b) 

1-t-butyl-4-methylcyclohexane

(e) 

2-cyclopentylheptane

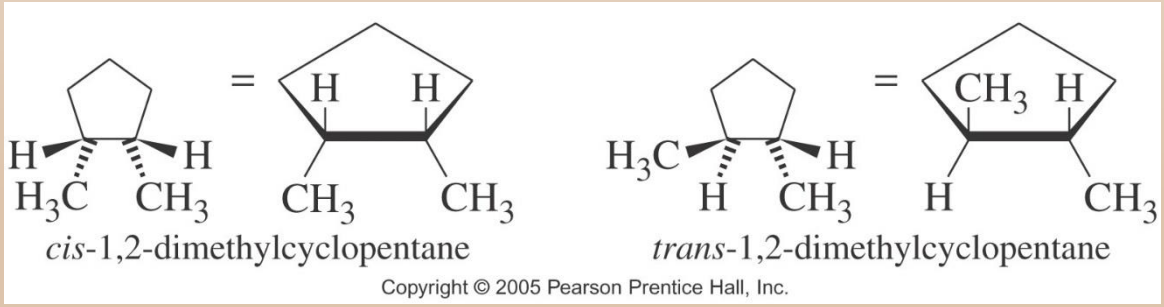
(c) 

1-ethyl-2,5-dimethylcyclohexane

(d) 

1-ethyl-1-methylcyclopropane

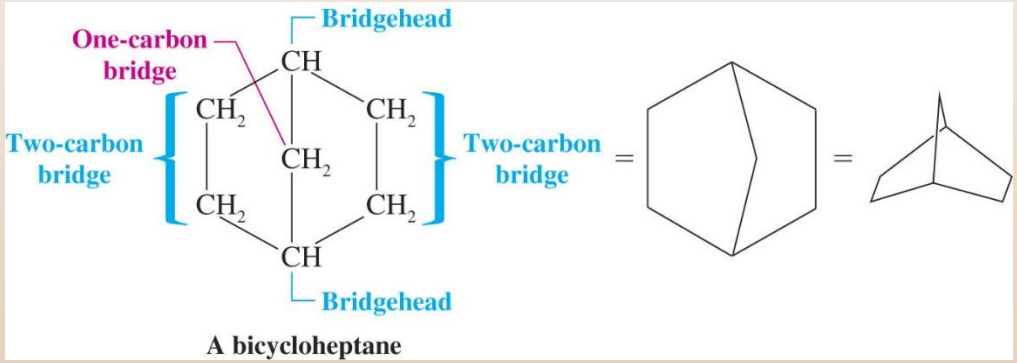
Cis-Trans Isomerism



- Cis: like groups on same side of ring
- Trans: like groups on opposite sides of ring

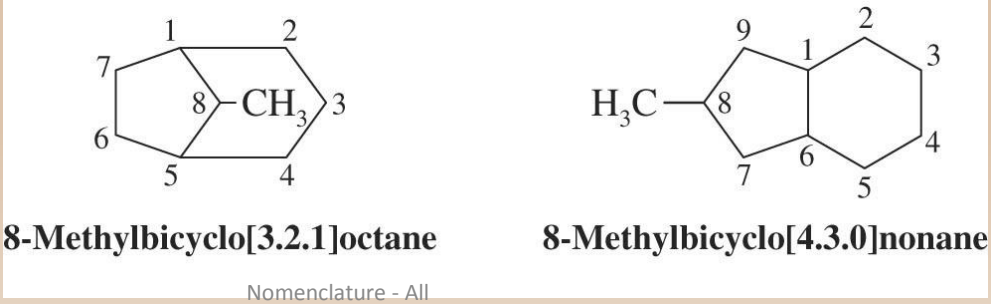
Bicyclic Compounds

- Bicyloalkanes contain 2 rings fused together (not connected by a bond)
- The alkane with the same number of total carbons is used as the parent and the prefix bicyclo- is used



Bicyclo [2.2.1] heptane

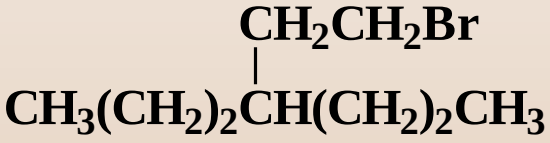
- The number of carbons in each bridge is included in the middle of the name in square brackets
- For substituents: number the largest ring; the substituent can get a large number.



Alkyl Halides

- Name as haloalkane.
- Choose the longest carbon chain, <u>even if</u> the halogen is not bonded to any of those C's.
- Use lowest possible numbers for position.

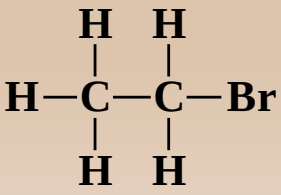
2-chlorobutan



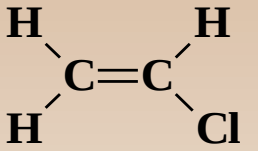
4-(2-bromoethyl)heptan

Classes of Halides

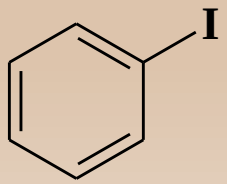
- Alkyl: Halogen, X, is directly bonded to sp^3 carbon.
- Vinyl: X is bonded to sp^2 carbon of alkene.
- Aryl: X is bonded to sp^2 carbon on benzene ring. Examples:



alkyl halide



vinyl halid



aryl halide

“Trivial” Names

- CH_2X_2 called methylene halide (e.g . CH_2Cl_2 is methylene chloride)
- CHX_3 is a haloform(e.g. $CHCl_3$ is chloroform)
- CX_4 is carbon tetrahalide. (e.g. CCl_4 is carbon tet)

More Classification of Alkyl Halides

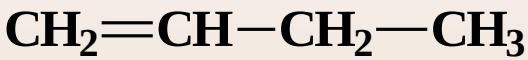
- Methyl halides: only one C, CH_3X
- Primary, Secondary and Tertiary
- Geminal and vicinal

Alkenes

- Parent is longest chain containing the double bond.
- -ane changes to -ene. (or -diene, -triene)
- Number the chain so that the double bond has the lowest possible number.
- In a ring, the double bond is assumed to be between carbon 1 and carbon 2.

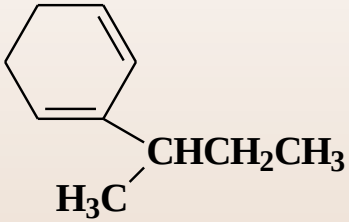
Examples

Note: Red names are new IUPAC



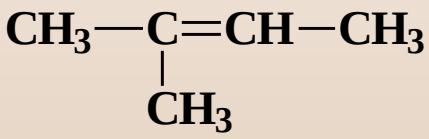
1-butene

but-1-ene



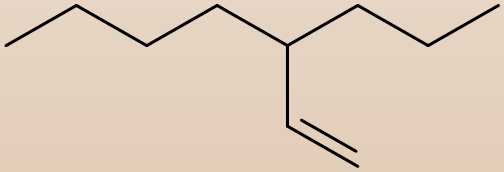
2-*sec*-butyl-1,3-cyclohexadiene

2-*sec*-butylcyclohexa-1,3-diene



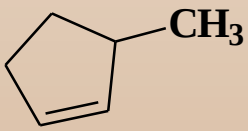
2-methyl-2-butene

2-methylbut-2-ene



3-*n*-propyl-1-heptene

3-*n*-propylhept-1-ene



3-methylcyclopentene

Alkene Substituents

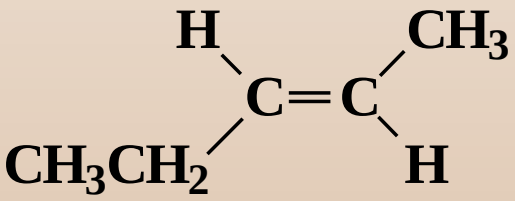
$= CH_2$	$- CH = CH_2$	$- CH_2 - CH = CH_2$
methylene (methylidene)	vinyl (ethenyl)	allyl (2-propenyl)

Common names for small molecules

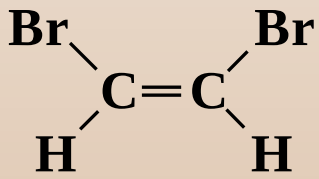
$CH_2=CH_2$	$CH_2=CH-CH_3$	$CH_2=C(CH_3)-CH_3$
ethylene	**propylene**	**isobutylene**

Cis-trans Isomerism

- Hydrogens on same side of double bond, alkene is cis.
- Hydrogens on opposite sides of double bond, alkene is trans.
- Cycloalkenes are assumed to be cis.
- Trans cycloalkenes are not stable unless the ring has at least 8 carbons.



trans-2-pentene
trans-pent-2-ene



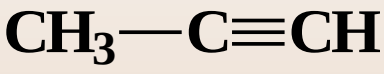
cis-1,2-dibromoethene

Alkynes

- Find the longest chain containing the triple bond.
- Change ***-ane*** ending to ***-yne***.
- Number the chain, starting at the end closest to the triple bond.
- Give branches or other substituents a number to locate their position.

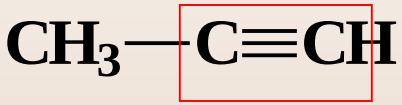
Examples

IUPAC Names



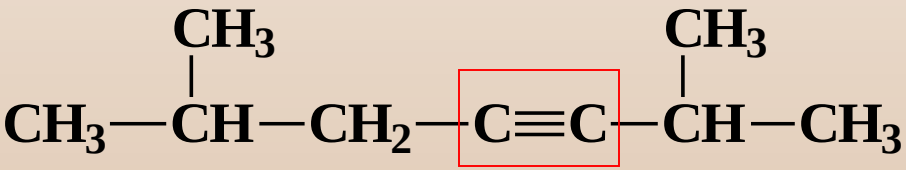
propyne

Common Names

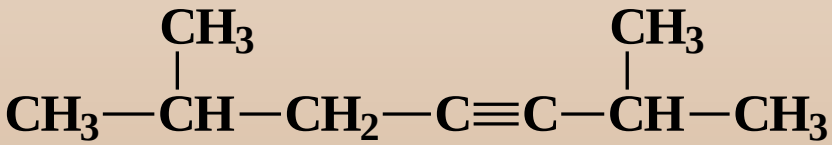


Methylacetylene
(terminal alkyne)

5-bromo-2-pentyne
5-bromopent-2-yne



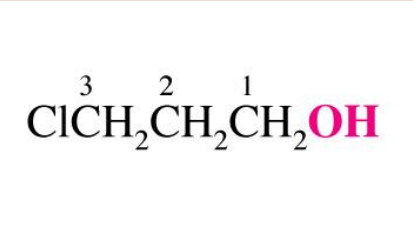
isobutylisopropylacetylene
(internal alkyne)



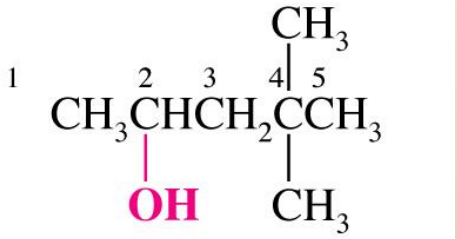
2,6-dimethyl-3-heptyne
2,6-dimethylpept-3-yne

Alcohols

- Select the longest chain containing the hydroxyl and change the suffix name of the corresponding parent alkane from -ane to -ol
- Number the parent to give the hydroxyl the lowest possible number
- The other substituents take their locations accordingly



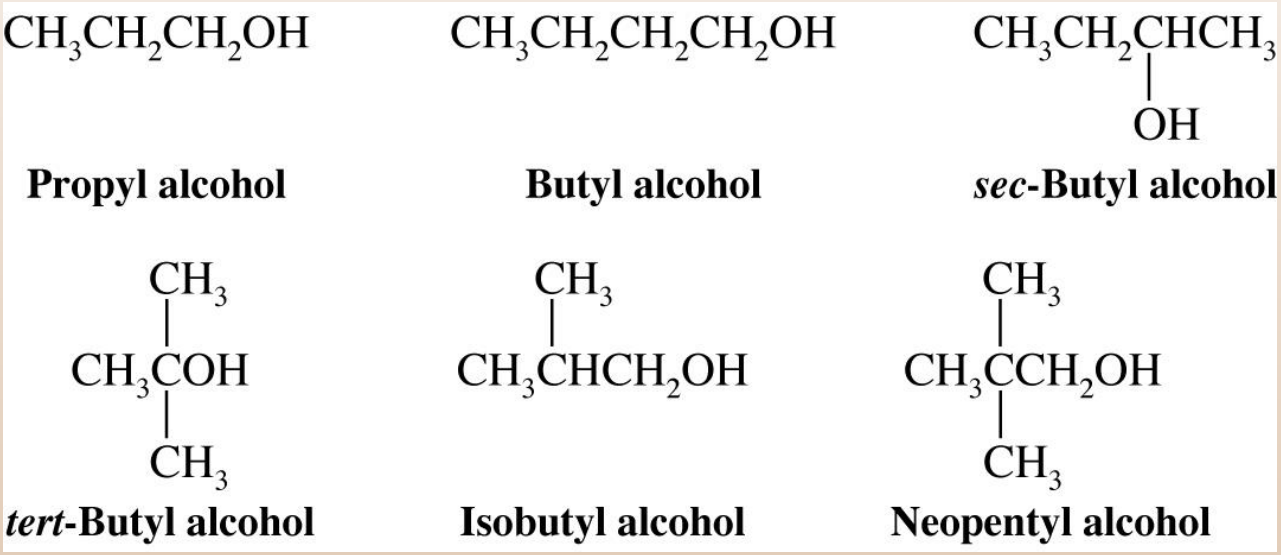
3-Chloro-1-propanol
or 3-chloropropan-1-ol

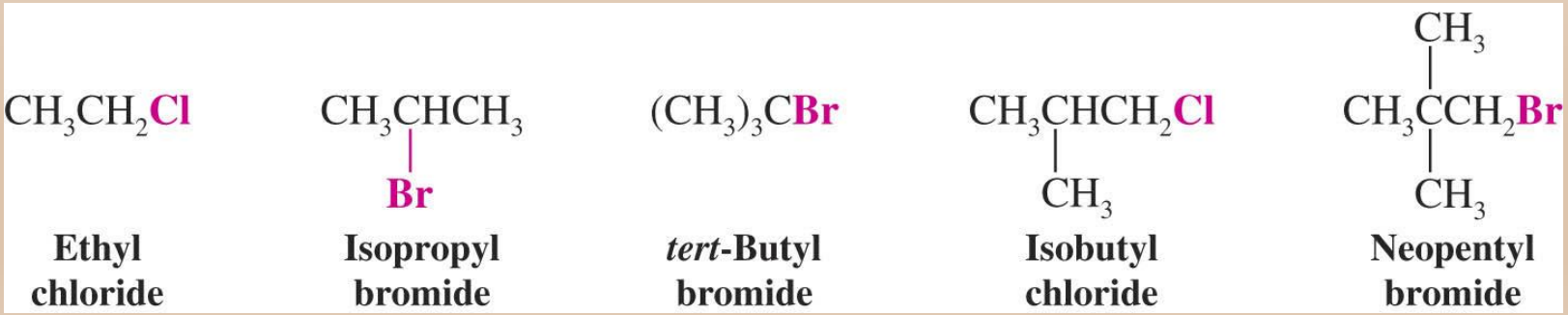


4,4-Dimethyl-2-pentanol
or 4,4-dimethylpentan-2-ol

Alcohols and Halides – Common Names

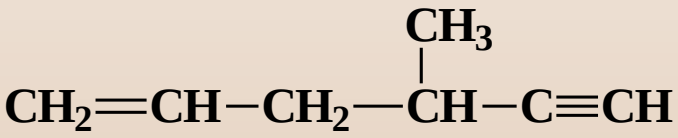
Common names of *simple alcohols* and *halides* still used and approved by IUPAC



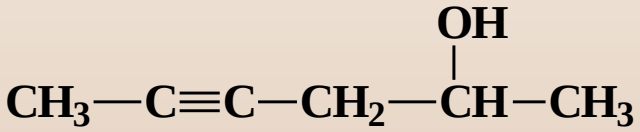


Additional Functional Groups

- All other functional groups, except ethers and halides have a higher priority than alkynes.
- For a complete list of naming priorities, look inside the back cover of your text.

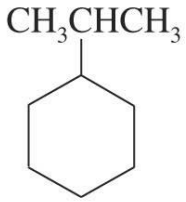


4-methyl-1-hexen-5-yne
4-methylhex-1-en-5-yne

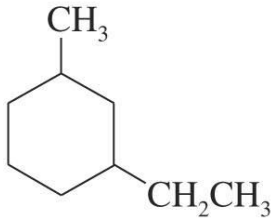


4-hexyn-2-ol
hex-4-yn-2-ol

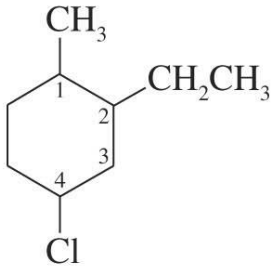
Solved Examples



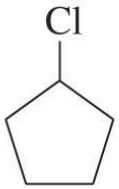
Isopropylcyclohexane



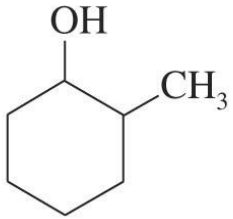
1-Ethyl-3-methylcyclohexane
(*not* 1-ethyl-5-methylcyclohexane)



4-Chloro-2-ethyl-1-methylcyclohexane
(*not* 1-chloro-3-ethyl-4-methylcyclohexane)

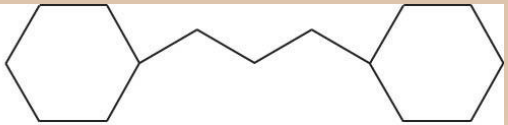


Chlorocyclopentane



2-Methylcyclohexanol

1-Cyclobutylpentane



1,3-Dicyclohexylpropane

Tips and Tricks for Writing Structural Isomers

- The following functional groups can have the same molecular formula.
  - Alkenes and Cycloalkanes
  - Alcohols and Ethers
  - Aldehydes and Ketones
  - Carboxylic acids and Esters
- It is very likely that you may have to draw more than one type of functional group for a given molecular formula in the different isomers.
- It is also likely that you may have more than one functional group in one compound!

Key Words/Concepts

- Naming alkanes, cycloalkanes and bicycloalkanes
- Constitutional isomers
- Cis and trans isomers in cycloalkanes
- Be able to write all types of representations (line structure, condensed structure and expanded structure)
- Know all the alkyl groups and the phenyl group