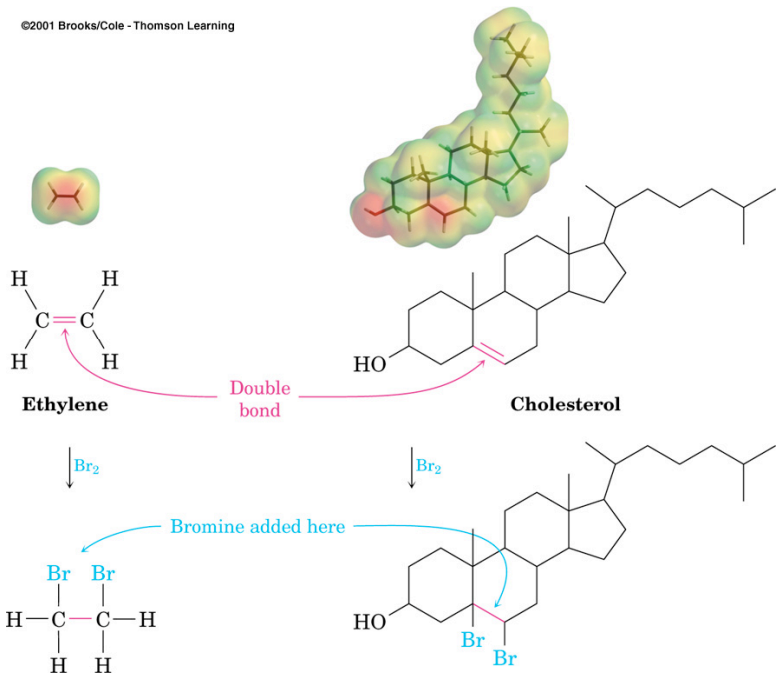
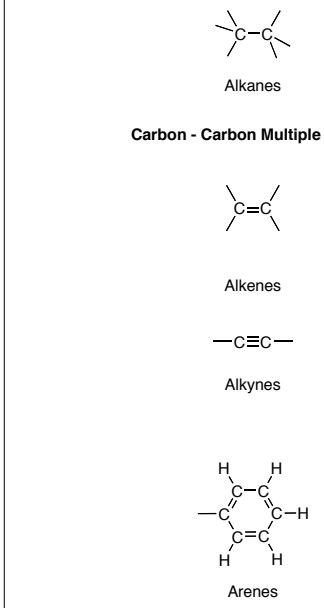
Chapter 3: Organic Compounds: Alkanes and Cycloalkanes

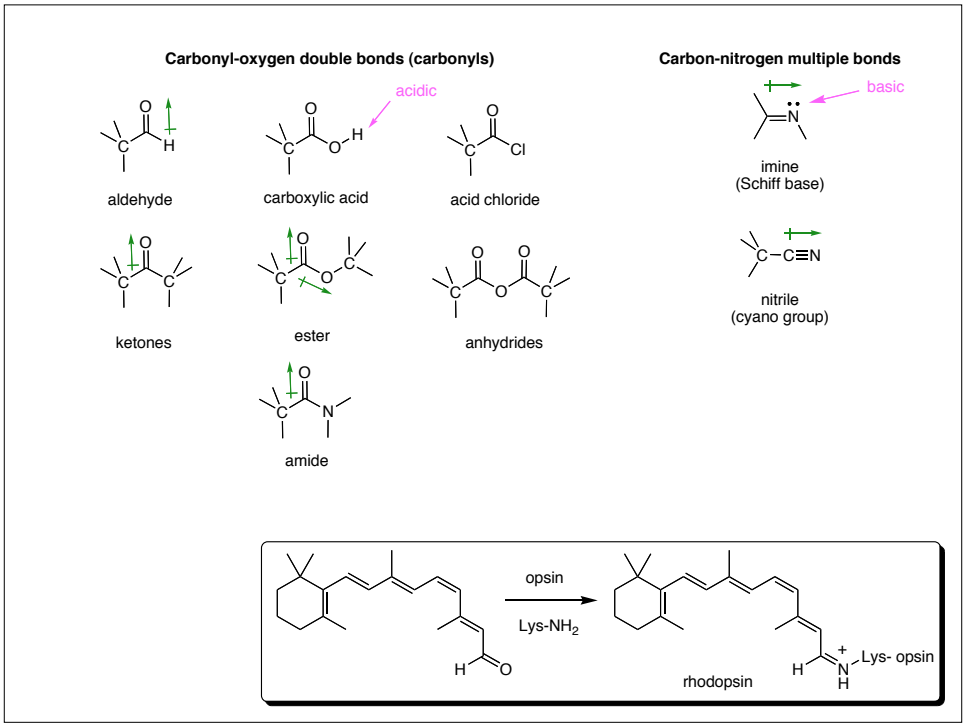
>11 million organic compounds which are classified into families according to structure and reactivity

Functional Group (FG): group of atoms which are part of a large molecule that have characteristic chemical behavior. FG's behave similarly in every molecule they are part of.

The chemistry of the organic molecule is defined by the function groups it contains




Alkanes
Carbon - Carbon Multiple Bonds
Alkenes
Alkynes
Arenes
Carbon-heteroatom single bonds
X= F, Cl, Br, I
Alkyl Halide
basic
amines
alcohols
acidic
ethers
thiols
sulfides
(disulfides)


Carbonyl-oxygen double bonds (carbonyls)
aldehyde
acidic
carboxylic acid
acid chloride
ketones
ester
anhydrides
amide
Carbon-nitrogen multiple bonds
basic
imine
(Schiff base)
nitrile
(cyano group)
opsin
Lys-NH2
rhodopsin
Lys- opsin

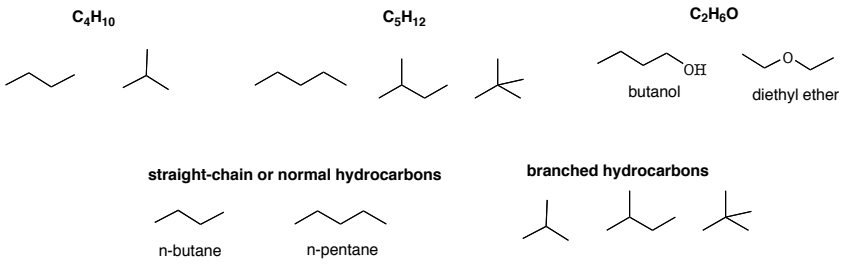
Alkanes and Alkane Isomers

Alkanes: organic compounds with only C-C and C-H single (□) bonds.
general formula for alkanes: $C_nH_{(2n+2)}$

Saturated hydrocarbons
Hydrocarbons: contains only carbon and hydrogen
Saturated" contains only single bonds

Isomers: compounds with the same chemical formula, but different arrangement of atoms

Constitutional isomer: have different connectivities (not limited to alkanes)



Systematic Nomenclature (IUPAC System)

Prefix-Parent-Suffix

Parent- number of carbons
Prefix- substituents
Suffix- functional groups

Naming Alkanes

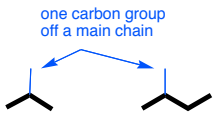
General Formula: $C_nH_{(2n+2)}$

suffix: -ane

Parent Names:

1	CH_4	**Meth**ane	CH_4
2	CH_3CH_3	**Eth**ane	C_2H_6
3	$CH_3CH_2CH_3$	**Prop**ane	C_3H_8
4	$CH_3(CH_2)_2CH_3$	**But**ane	C_4H_{10}
5	$CH_3(CH_2)_3CH_3$	**Pent**ane	C_5H_{12}
6	$CH_3(CH_2)_4CH_3$	**Hex**ane	C_6H_{14}
7	$CH_3(CH_2)_5CH_3$	**Hept**ane	C_7H_{16}
8	$CH_3(CH_2)_6CH_3$	**Oct**ane	C_8H_{18}
9	$CH_3(CH_2)_7CH_3$	**Non**ane	C_9H_{20}
10	$CH_3(CH_2)_8CH_3$	**Dec**ane	$C_{10}H_{22}$

Alkyl substituents (group): carbon chains which are a substructue of a molecule



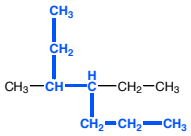
R= Rest of the molecule (mainchain)

1	CH_3-R	**Meth**yl
2	CH_3CH_2-R	**Eth**yl
3	$CH_3CH_2CH_2$-R	**Prop**yl
4	$CH_3(CH_2)_2CH_2$-R	**But**yl
5	$CH_3(CH_2)_3CH_2$-R	**Pent**yl
6	$CH_3(CH_2)_4CH_2$-R	**Hex**yl
7	$CH_3(CH_2)_5CH_2$-R	**Hept**yl
8	$CH_3(CH_2)_6CH_2$-R	**Oct**yl
9	$CH_3(CH_2)_7CH_2$-R	**Non**yl
10	$CH_3(CH_2)_8CH_2$-R	**Dec**yl

Rules for Systematic Nomenclature of Alkanes

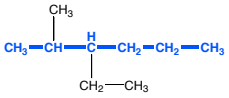
1. *Find the parent chain*

a. Identify the longest continuous carbon chain as the parent chain.

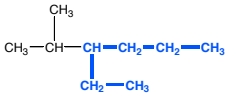


7 carbons = hept-

b. If more than one different chains are of equal length (number of carbons), choose the one with the greater number of branch points (substituents) as the parent.



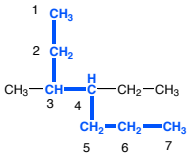
2 branch pts.



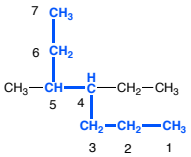
1 branch pt.

2. *Numbering the carbons of the parent chain*

a. Number the carbon atoms of the parent chain so that any branch points have the lowest possible number

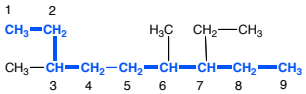


branch pts. at carbons 3 and 4

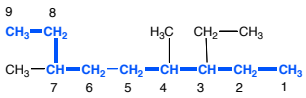


branch pts. at carbons 4 and 5

b. If there is branching equidistant from both ends of the parent chain, number so the second branch point has the lowest number.

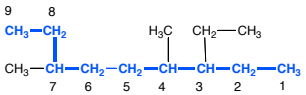


branch pts. at carbons 3, 6, 7



branch pts. at carbons 3,4,7

3. *Substituents*
    a. Identify and number the substituents and list them in alphabetical order.



Parent C-9 = nonane
3- ethyl
4-methyl
7-methyl
} 4,7-dimethyl

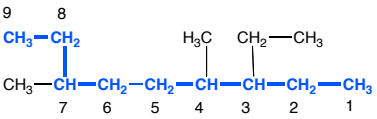
    b. If there are two substituents on the same carbon, assign them the same number.

4. *Write out the name*
    a. Write out the name as a single word:
        hyphens (-) separate prefixes
        commas (,) separate numbers
    b. Substituents are listed in alphabetical order

4c. If two or more identical substituents are present use the prefixes:

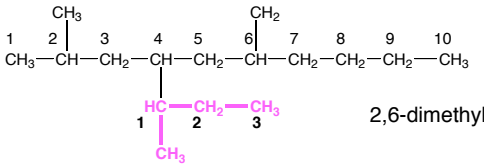
di- for two
tri- for three
tetra- for four

note: these prefixes (di-, tri-, tetra-, etc.) are not used for alphabetizing purposes



3- ethyl-4,7-dimethylnonane

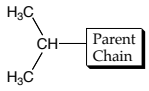
5. *Complex Substituents (substituents with branching)*
   a. Named by applying the four previous rules with some modification
   b. Number the complex substituent separately from the parent. Begin numbering at the point of attachment to the parent chain.
   c. Complex substituents are set off by parenthesis.



2,6-dimethyl-4-(1-methylpropyl)decane

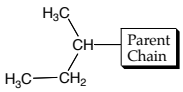
Nonsystematic (trivial) Names:

3-carbons:

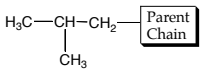


Isopropyl-
(1-methylethyl)

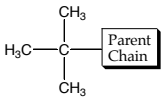
4-Carbons:



sec-butyl-
(1-methylpropyl)

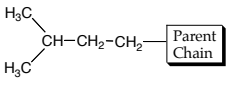


Isobutyl-
(2-methylpropyl)

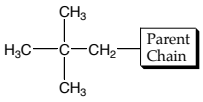


tert-butyl-
(1,1-dimethylethyl)

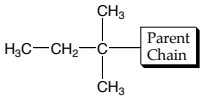
5- Carbons:



Isopentyl-, isoamyl
(3-methylbutyl)



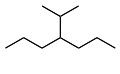
neopentyl-
(2,2-dimethylpropyl)



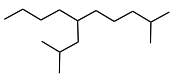
tert-pentyl-, tert-amyl
(1,1-dimethylpropyl)

Alphabetizing trivial names:

Iso- and neo are part of the alkyl group name and are used for alphabetizing.
sec- and tert- are not included in the alphabetical order.



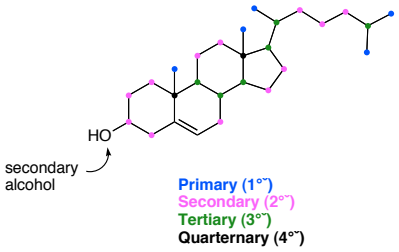
4-(1-methylethyl)heptane
-or-
4-Isopropylheptane



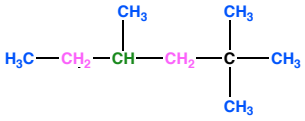
2-methyl-6-(2-methylpropyl)decane
-or-
6-Isobutyl-2-methyldecane

Degrees of Substitution

Primary (1°) Carbon: carbon which is bonded to only one other carbon
Secondary (2°) Carbon: carbon which is bonded to two other carbons
Tertiary (3°) Carbon: carbon which is bonded to three other carbons
Quarternary (4°) Carbon: carbon whohc is bonded to four other carbons

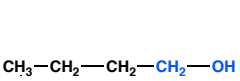


1° Hydrogens- hydrogens on a primary carbon. $-CH_3$ (methyl group)
2° Hydrogens- hydrogens on a secondary carbon. $-CH_2-$ (methylene group)
3° Hydrogens- hydrogens on a tertiary carbon. CH (methane group)

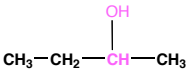


methyl group: 1° hydrogens
methylene group: 2° hydrogens
methine group: 3° hydrogens

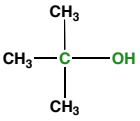
Applied to other functional groups:



n-butanol
1° alcohols



sec-butanol
2° alcohol



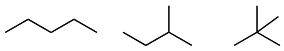
tert-butanol
3° alcohol

Alkanes show: regular increase in bp and mp as the molecular weight increase. Branching lowers the bp or alkanes

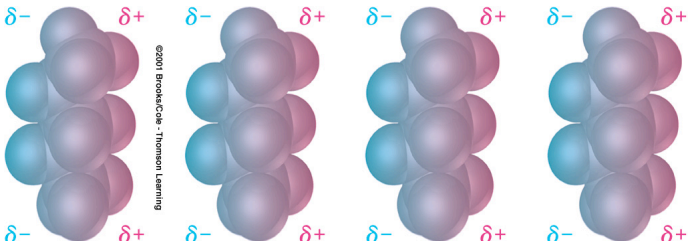
n-pentane bp= 36.1 °C

i-penatane bp= 27.9 °C

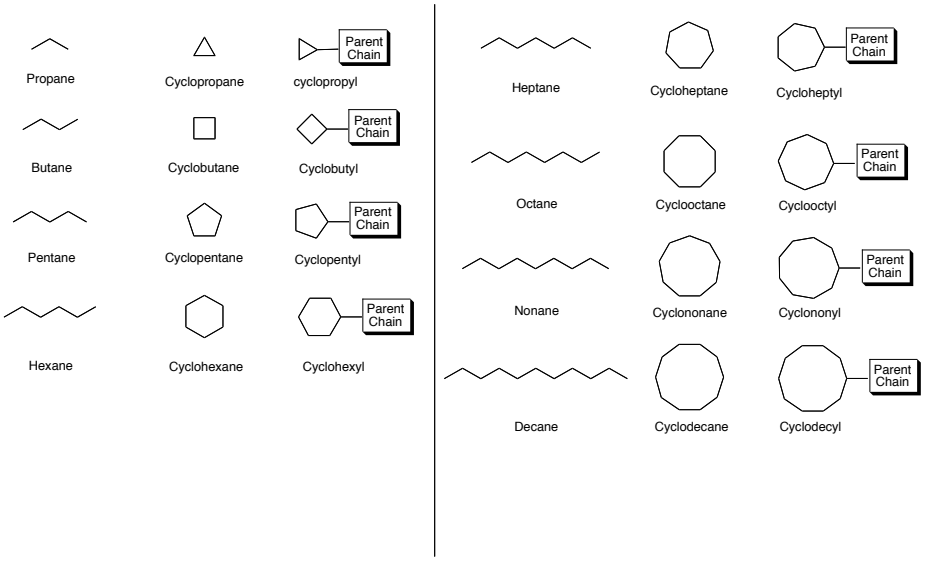
neo-pentane bp= 9.5°C



Van der Waals Forces: small temporary dipoles that are a result of a Distortion of the electron clouds. There is an attraction between molecules as result of these temporary dipoles



Cycloalkanes

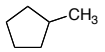


Naming Cycloalkanes General Formula: $C_nH_{(2n)}$

1. Parent Chain

a. Use the cycloalkane as the parent chain if it has a greater number of carbons than any alkyl substituent.

b. If an alkyl chain off the cycloalkane has a greater number of carbons, then use the alkyl chain as the parent and the cycloalkane as a **cycloalkyl-** substituent.

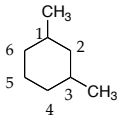


Methylcyclopentane

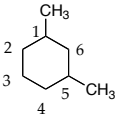
2-Cyclopropylbutane

2. Numbering the Cycloalkane

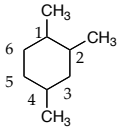
a. When numbering the carbons of a cycloalkane, start with a substituted carbon so that the substituted carbons have the lowest numbers (sum).



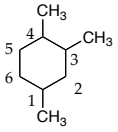
1,3-Dimethylcyclohexane



-not-
1,5-Dimethylcyclohexane

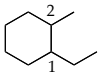


1,2,4-Trimethylcyclohexane
(1 + 2 + 4 = 7)

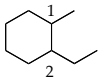


-not-
1,3,4-Trimethylcyclohexane
(1 +3 + 4 = 8)

2. b. When two or more different substituents are present, number according to alphabetical order.



1-Ethyl-2-methylcyclohexane



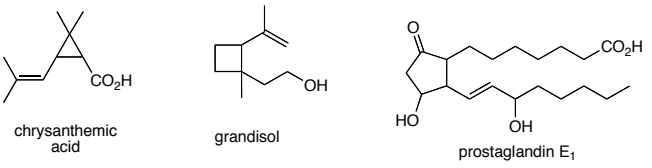
-not-
2-Ethyl-1-methylcyclohexane

3. Halogen Substituents

Halogen substituents are treated exactly like alkyl groups:

-F	fluoro-
-Cl	chloro-
-Br	bromo-
-I	iodo-

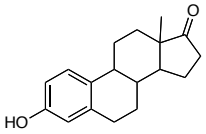
1-Chloro-2-methylcyclobutane



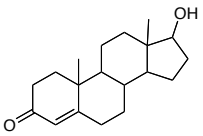
chrysanthemic acid

grandisol

prostaglandin E_1



esterone



testosterone