Lacture1

ORGANIC COMPOUNDS

م.م زينب يحيى كاظم

organic compounds contain only two elements hydrogen carbon. **organic compounds**: organic chemistry is the chemistry of carbon and only a few other elements-chiefly, hydrogen, oxygen, nitrogen, sulfur, halogens, and phosphorus (from 116 elements).

Note: In the early days of chemistry, scientists though organic compounds were those produced by living organisms and they could not synthesize any organic compound by starting with only inorganic compounds. In 1828, Friedrich Wöhler synthesized the first organic compound in his laboratory (urea).

$$\underset{\text{Ammonium chloride}}{\mathbf{NH_4Cl}} + \underset{\text{Silver cyanate}}{\mathbf{AgNCO}} \xrightarrow{\text{heat}} \underset{\text{Urea}}{\mathbf{H_2N\text{-}\overset{\overset{\displaystyle O}{\|}}{C}\text{-}NH_2}} + \underset{\text{Silver chloride}}{\mathbf{AgCl}}$$

Why organic chemistry

we can find organic compounds everywhere around us (foods, flavors, fragrances, medicines, toiletries, plastic, paints, our body, and etc.). Chemistry have discovered or synthesized more than 10 million of organic compounds. However, 1.7 million inorganic compounds are discovered or synthesized (85% of all known compounds are organic compounds).

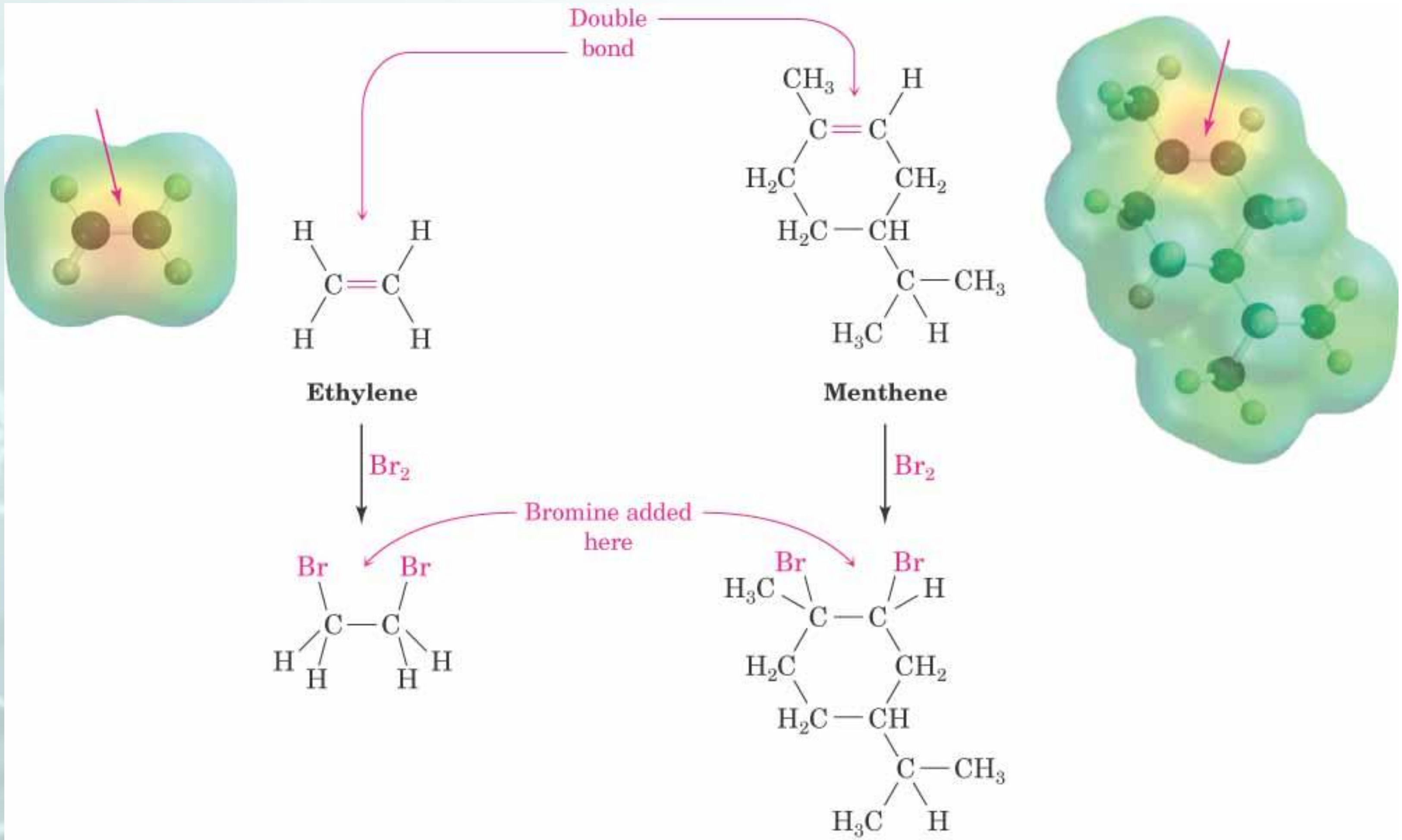
properties of organic compounds:

1. They contain carbon atom.
2. Bonding is almost entirely covalent (covalent compounds).
3. They have low boiling points and low melting points.
4. They are flammable (almost all burn).
5. They are soluble in nonpolar compounds and most are insoluble in water.
6. Many are gases, liquids, or solids.

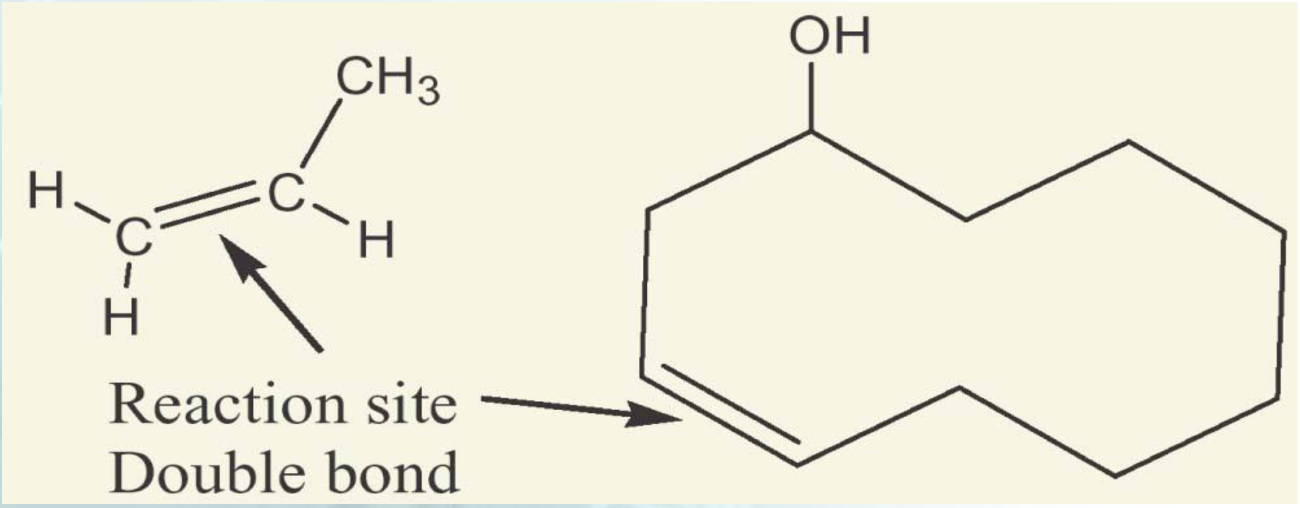
Functional group

an atom or group of atoms within a molecule that shows a characteristic set of predictable physical and chemical behaviors.

- **Functional group -** collection of atoms at a site within a molecule with a common bonding pattern
- The group reacts in a typical way, generally independent of the rest of the molecule
- For example, the double bonds in simple and complex alkenes react with bromine in the same way


Double bond
Ethylene
Menthene
Br2
Br2
Bromine added here
Br
Br
Br
Br

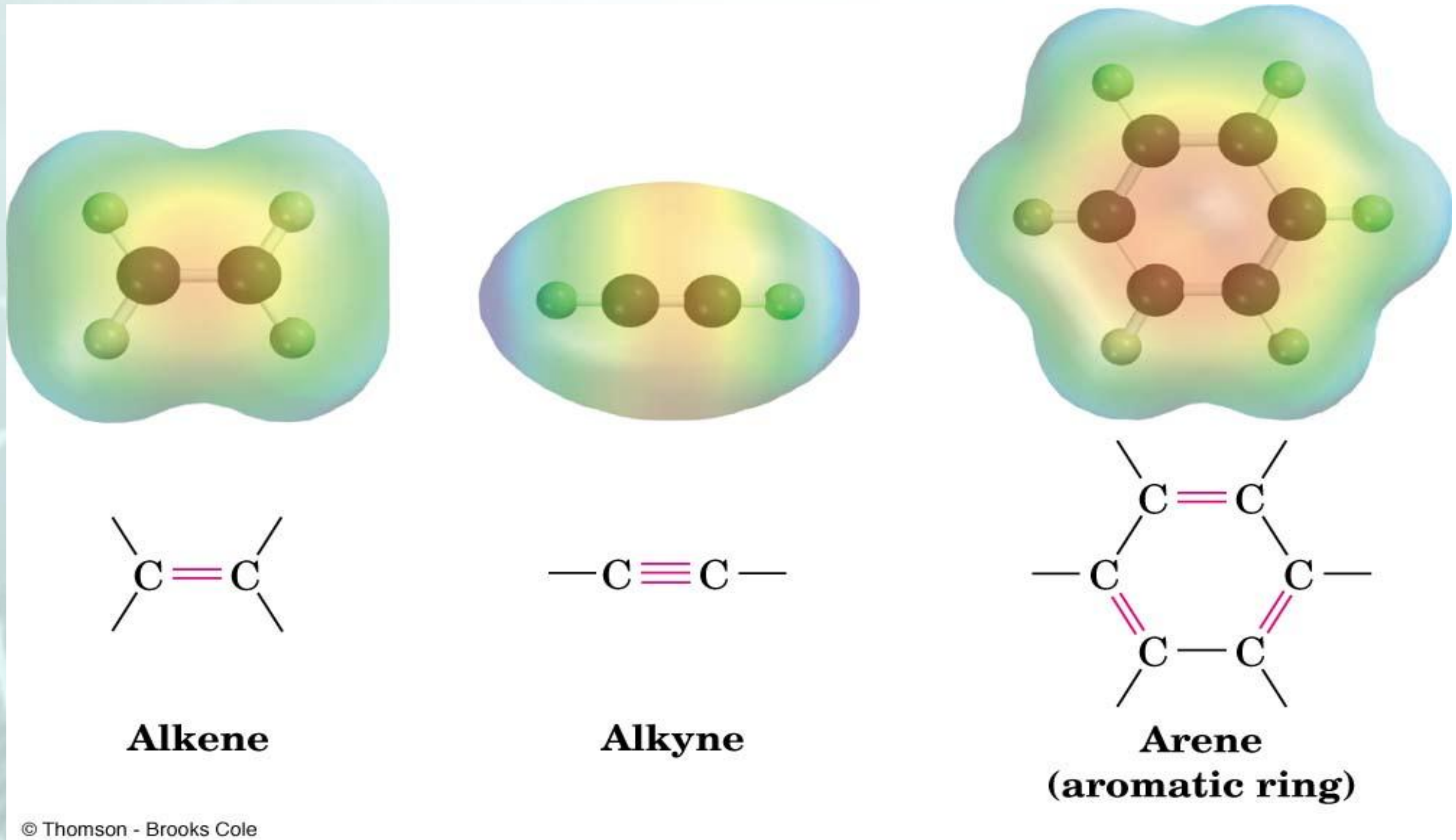
Double Bond as Functional Group



Types of Functional Groups: Multiple Carbon–Carbon Bonds

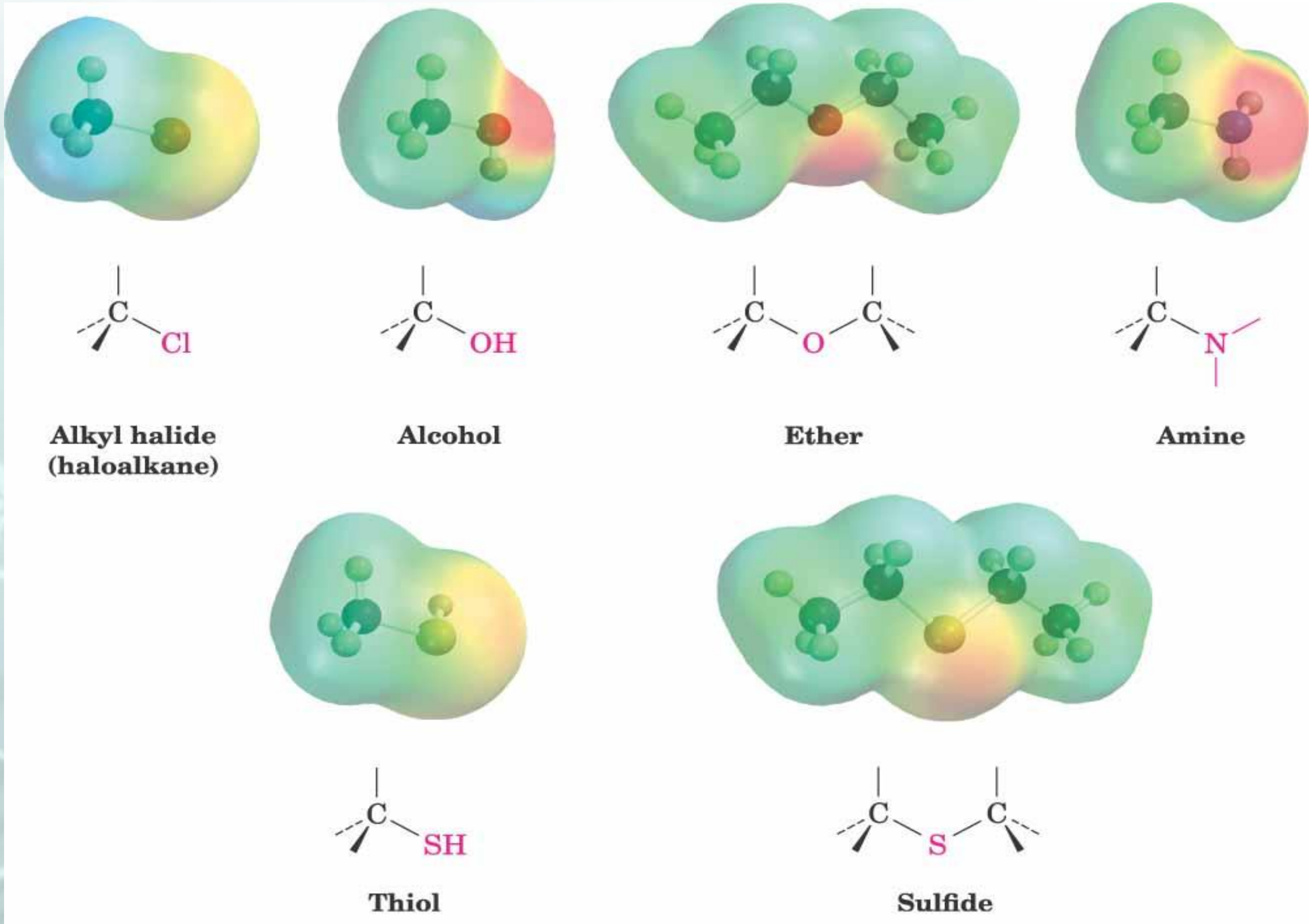
- *Alkenes* have a C-C double bond
- *Alkynes* have a C-C triple bond
- *Arenes* (or aromatic hydrocarbons) have special bonds that are represented as alternating single and double C-C bonds in a six-membered ring

Multiple Carbon–Carbon Bonds



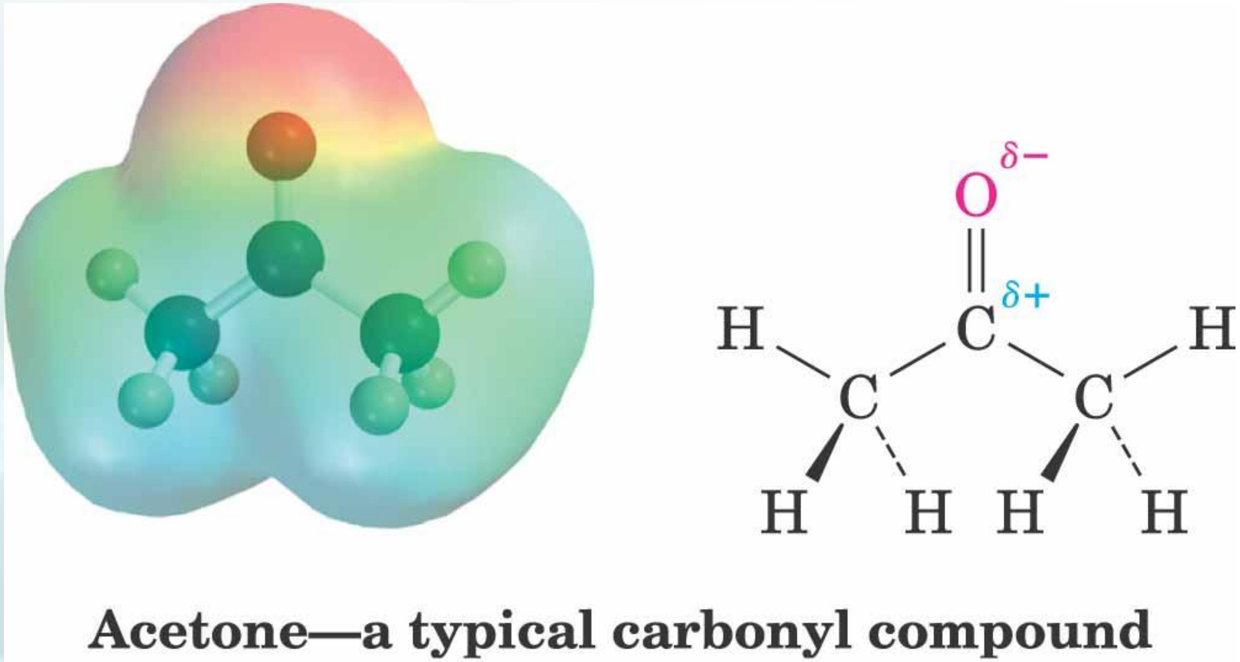
Functional Groups with Carbon Singly Bonded to an Electronegative Atom

- *Alkyl halide:* C bonded to halogen (C-X)
- *Alcohol: C* bonded O of a hydroxyl group (C-OH)
- *Ether:* Two C's bonded to the same O (C-O-C)
- *Amine:* C bonded to N (C-N)
- *Thiol:* C bonded to SH group (C-SH)
- *Sulfide:* Two C's bonded to same S (C-S-C)
- Bonds are polar, with part positive charge on C (δ+) and part negative charge (δ–) on electronegative atom

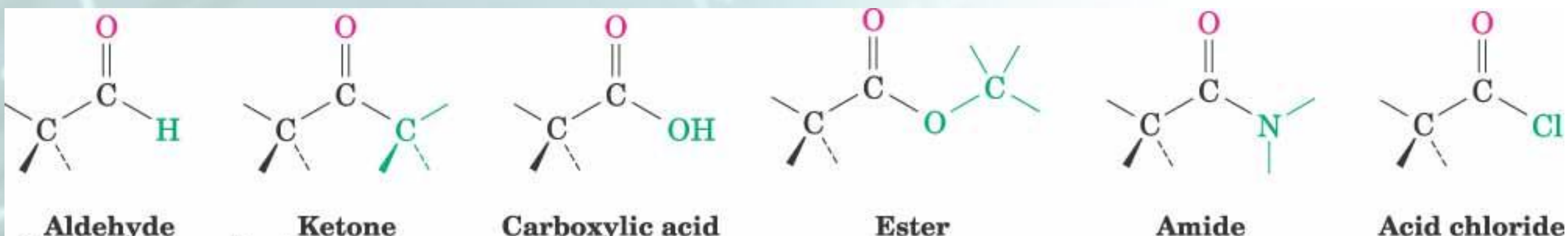

Cl
OH
O
N
SH
S
Alkyl halide
(haloalkane)
Alcohol
Ether
Amine
Thiol
Sulfide

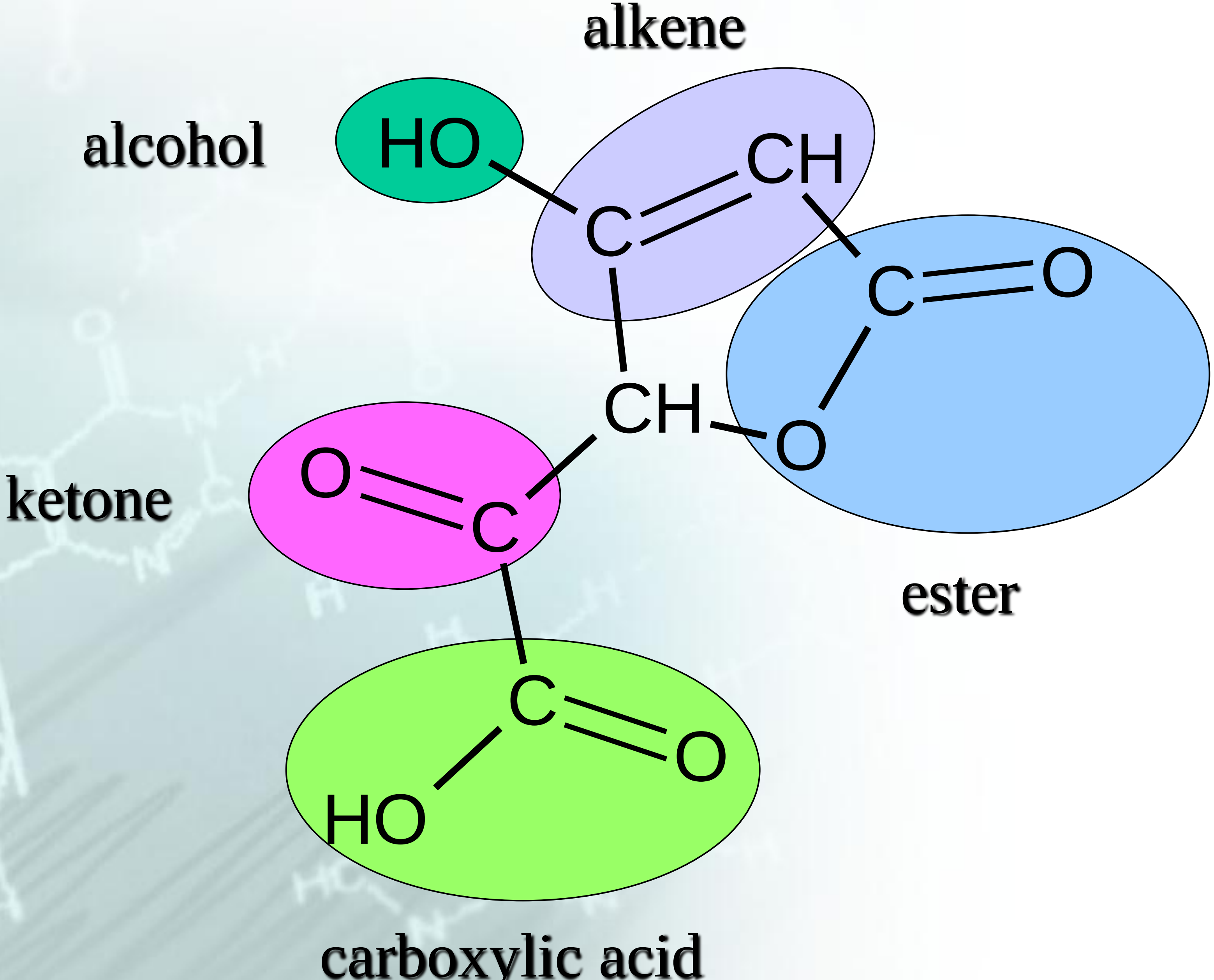
Groups with a Carbon–Oxygen Double Bond (Carbonyl Groups)

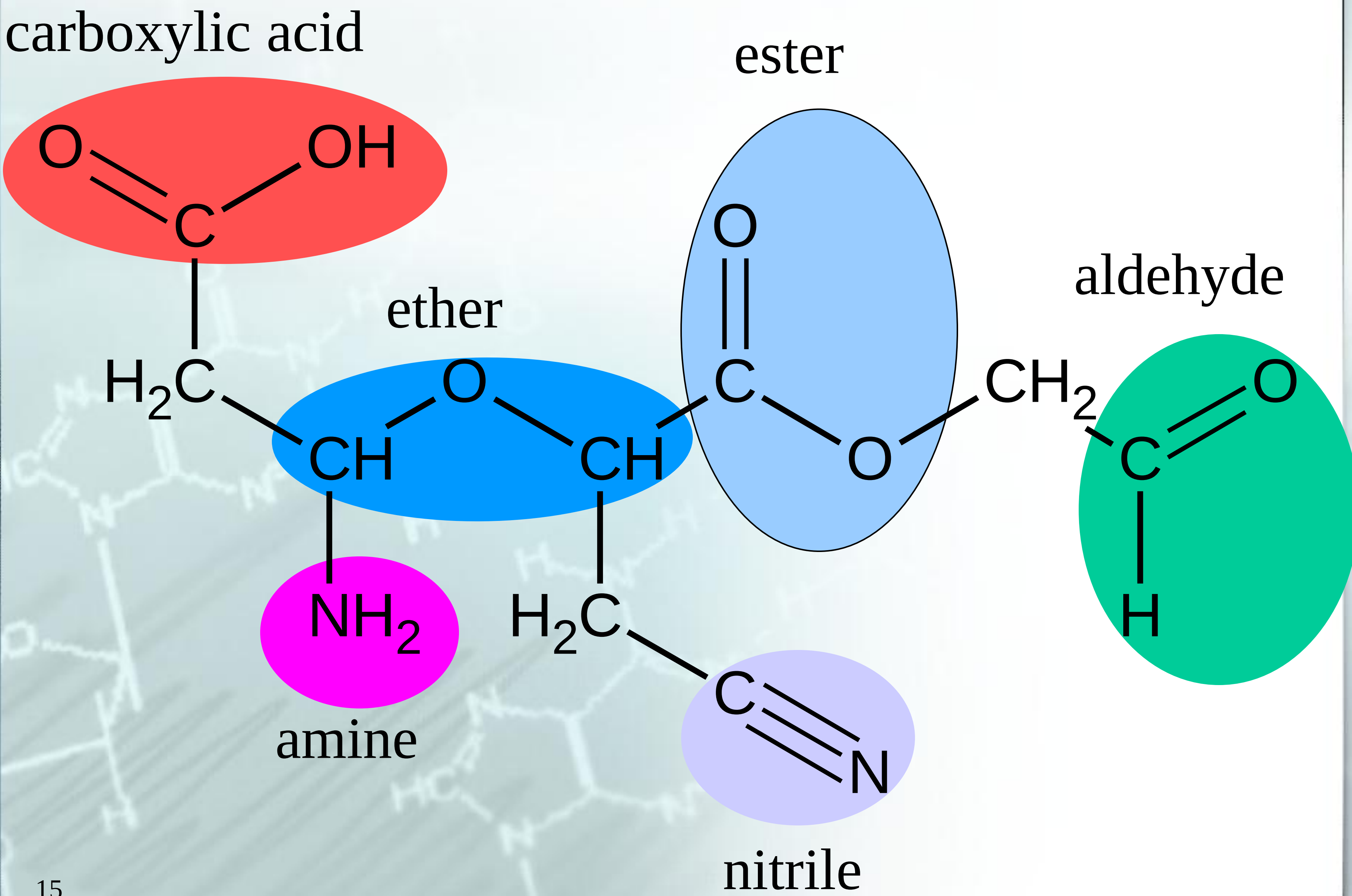
- *Aldehyde:* one hydrogen bonded to C=O
- *Ketone:* two C's bonded to the C=O
- *Carboxylic acid:* -OH bonded to the C=O
- *Ester:* C-O bonded to the C=O
- *Amide:* C-N bonded to the C=O
- *Acid chloride:* Cl bonded to the C=O
- Carbonyl C has partial positive charge (δ+)
- Carbonyl O has partial negative charge (δ-).



Acetone—a typical carbonyl compound




alkene
alcohol
HO
CH
C
C
O
CH
O
ketone
O
C
ester
C
O
HO
carboxylic acid


carboxylic acid
ester
aldehyde
ether
amine
nitrile
O
OH
C
O
C
O
CH$_2$
C
O
H
H$_2$C
CH
O
CH
NH$_2$
H$_2$C
C
N

Hydrocarbons

Hydrocarbons are divided into two groups:

1. Saturated hydrocarbon: a hydrocarbon that contains only carbon-carbon single bonds (alkanes, also called Aliphatic hydrocarbons). Saturated in this context means that each carbon in the hydrocarbon has the maximum number of hydrogen atoms bonded to it.

2. Unsaturated hydrocarbon: a hydrocarbon that contains one or more carbon-carbon double bonds, triple bonds, or benzene rings.

Hydrocarbons

Large family of organic compounds

Composed of only carbon and hydrogen

Saturated hydrocarbons

Unsaturated hydrocarbons

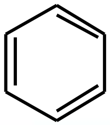
Alkanes

Alkenes, Alkynes & Aromatics

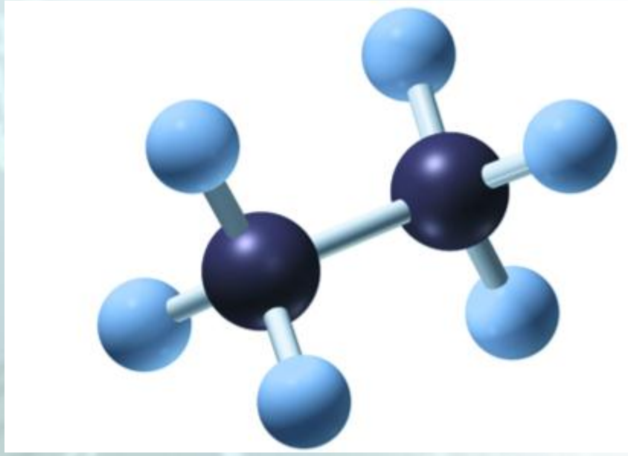
C - C

C = C

C≡C



Alkanes



Alkanes: Are Saturated hydrocarbons. These compounds divide into two type

1- open chain in alkanes

2- cyclic alkanes

Alkanes all have very similar structures.

They have a CH_3 at each end of the molecule.

What differs is the number of CH_2 groups between the two ends.

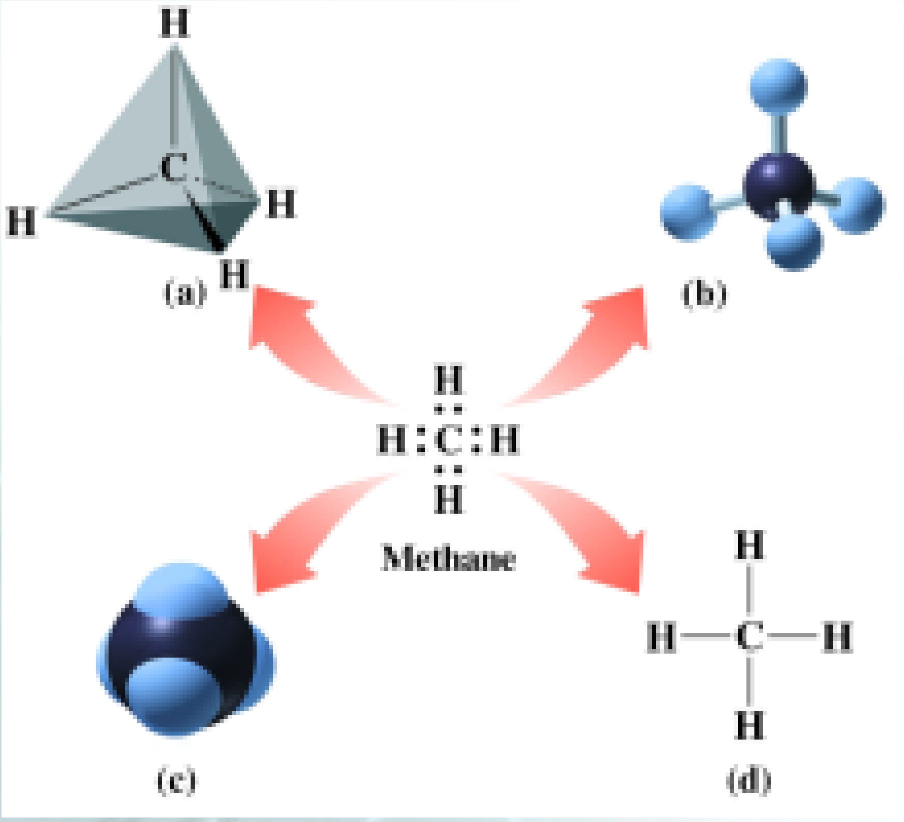
These all consist of carbon and hydrogen only and every carbon has four single covalent bonds.

It is possible to build up a series by simply adding an extra CH_2 group

This leads to a general formula of $\mathbf{C_nH_{2n+2}}$

Methane

Tetrahedral

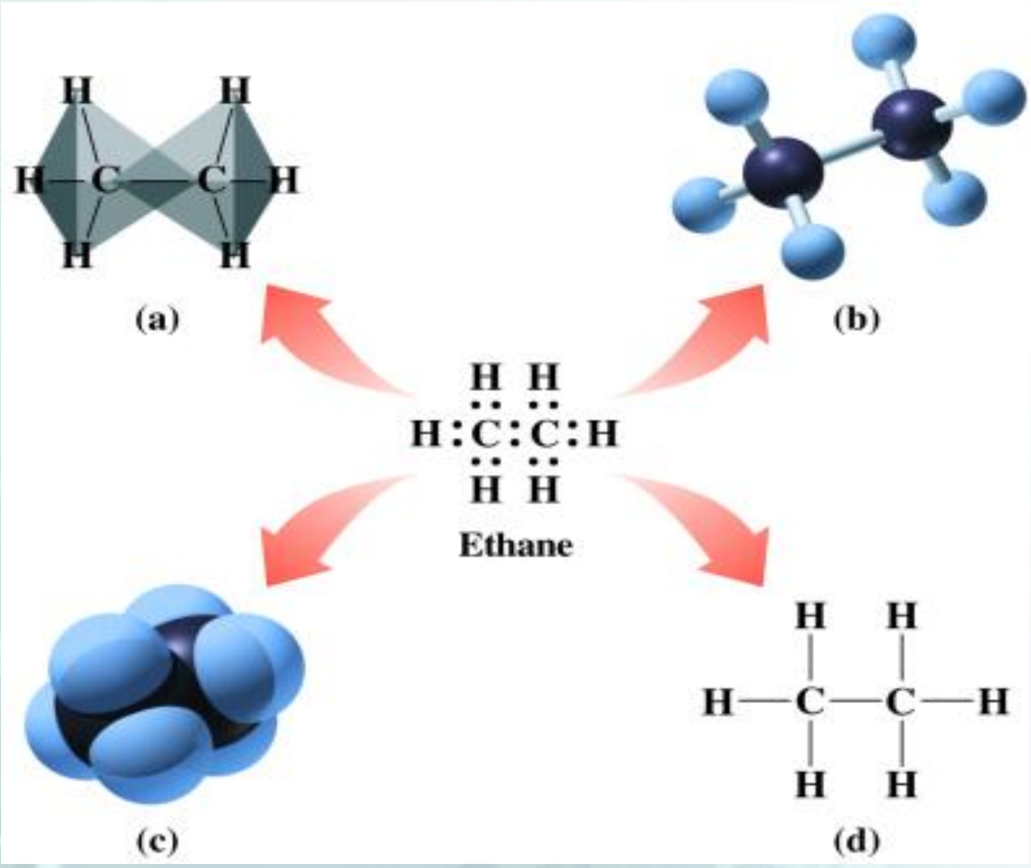


Molecular formula CH_4

Expanded structural formula:

showing each bond line.

Ethane



C_2H_6 Molecular formula

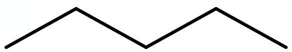
Expanded structural formula

$CH_3 - CH_3$

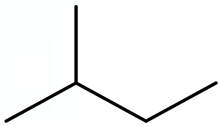
Condensed structural formula: with each carbon atom and its attached hydrogen atoms.

Common name

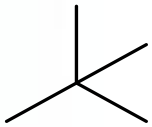
C_5H_{12} pentane(s)

$CH_3CH_2CH_2CH_2CH_3$ *n-pentane* 

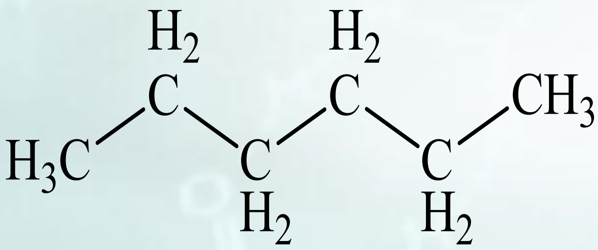
$$
\begin{array}{c}
\qquad\qquad CH_3 \\
\qquad\qquad | \\
H_3C\diagdown_{\underset{H_2}{C}}\diagup CH\diagdown_{CH_3}
\end{array}
$$

isopentane 

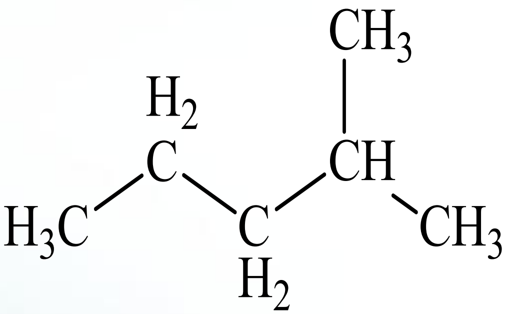
$$
\begin{array}{c}
CH_3 \\
| \\
H_3C-C-CH_3 \\
| \\
CH_3
\end{array}
$$

neopentane 

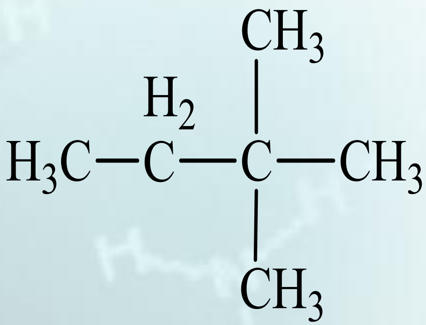
hexanes C_6H_{14} common names



n-hexane



isohexane



neohexane

IUPAC rules for naming alkanes:

1. parent chain = longest continuous carbon chain → “alkane”.
2. branches on the parent chain are named as “alkyl” groups.
3. number the parent chain starting from the end that gives you the lower number for the first branch (principle of lower number).
4. assign “locants” to the alkyl branches.
5. if an alkyl group appears more than once use prefixes: di, tri, tetra, penta…; each alkyl group must have a locant!
6. the name is written as one word with the parent name last. The names and locants for the alkyl branches are put in alphabetic order (ignore all prefixes except iso) separating numbers from numbers with commas and letters from numbers with hyphens.

IUPAC nomenclature (Geneva, 1920)
names of radicals (alkyl groups):

CH_3 **Methyl**

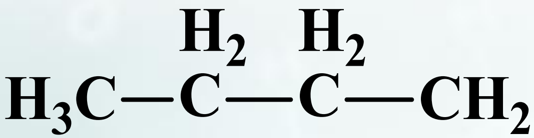
$H_3C{-}Cl$ Methyl chloride

$H_3C{-}OH$ Methyl alcohol, etc.

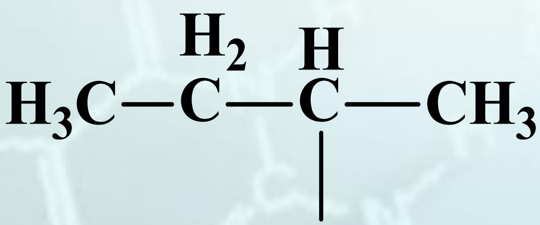
$H_3C{-}CH_2$ **Ethyl**

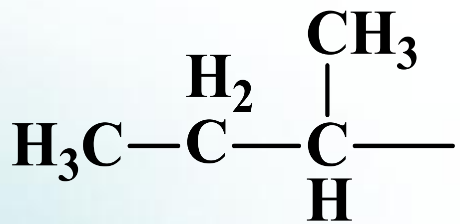
$H_3C{-}\overset{H_2}{C}{-}CH_2$ **n-propyl**

$H_3C{-}\overset{H}{\underset{|}{C}}{-}CH_3$ **Isopropyl**

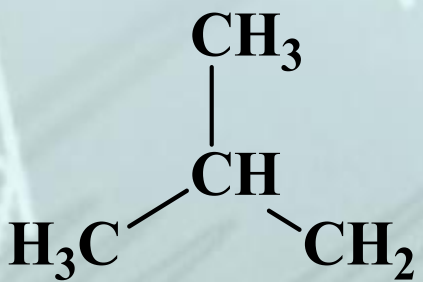


n-butyl

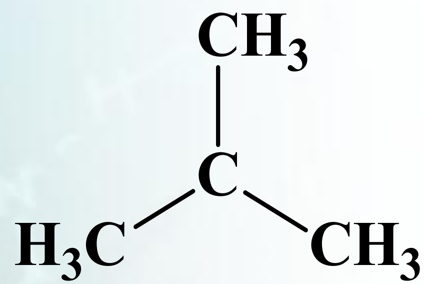




sec-butyl



isobutyl



tert-butyl

Two isomers of butane C_4H_{10}:

$CH_3CH_2CH_2CH_3$ *n*-butane

bp 0 ^oC
mp –138 ^oC
d 0.622 g/cc

$$\begin{array}{l} \quad\; CH_3 \\ CH_3CHCH_3 \end{array}$$

isobutane

bp -12 ^oC
mp -159 ^oC
d 0.604 g/cc

n-propyl bromide

$CH_3CH_2CH_2Br$

$BrCH_2CH_2CH_3$

$$\begin{array}{l} CH_3 \\ | \\ CH_2CH_2Br \end{array}$$

isopropyl bromide

$$\begin{array}{lcl} CH_3 & CH & CH_3 \\ & | & \\ & Br & \end{array}$$

$$\begin{array}{lc} & CH_3 \\ & | \\ CH_3 & CHBr \end{array}$$

$$\begin{array}{l} CH_3 \\ | \\ CHBr \\ | \\ CH_3 \end{array}$$

n-butyl chloride

$CH_3CH_2CH_2CH_2Cl$ $\qquad$ $CH_3CH_2CH_2\underset{\overset{|}{Cl}}{C}H_2$ $\qquad$ $ClCH_2CH_2CH_2CH_3$

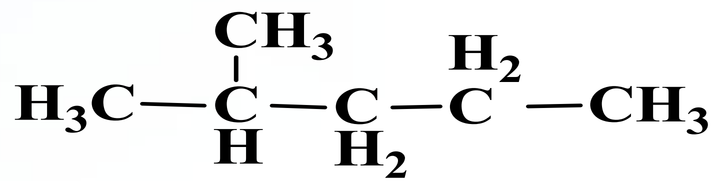
sec-butyl chloride

$CH_3\underset{\overset{|}{Cl}}{C}HCH_2CH_3$ $\qquad$ $CH_3CH_2\underset{\overset{|}{Cl}}{C}HCH_3$ $\qquad$ $CH_3CH_2\overset{\underset{|}{CH_3}}{C}H{-}Cl$

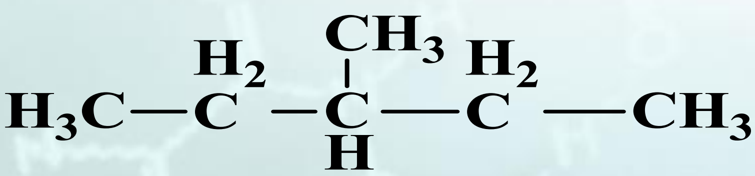
Hexanes C_6H_{14} IUPAC names

$CH_3CH_2CH_2CH_2CH_2CH_3$

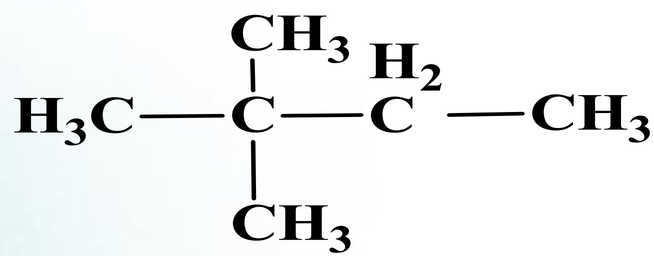
(n-Hexane)



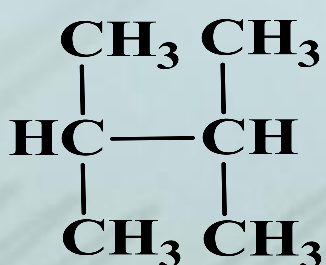
(isohexane)
2-methylpentane



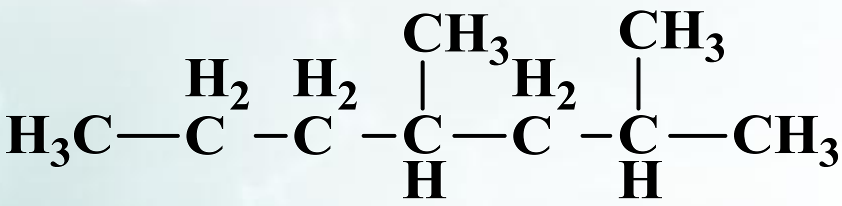
(no common name)
3-methylpentane



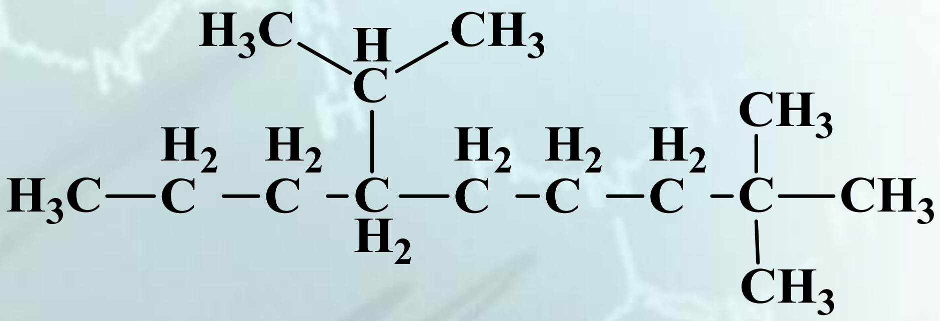
(neohexane)
2,2-dimethylbutane



(no common name)
2,3-dimethylbutane



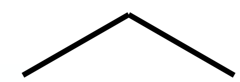
2,4-dimethylheptane



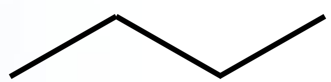
6-isopropyl-2,2-dimethylnonane

Line-angle Formula

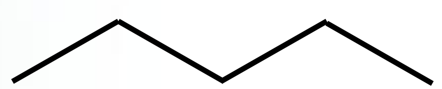
Propane $CH_3\text{-}CH_2\text{-}CH_3$



Butane $CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_3$



Pentane $CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3$



Naming Substituents

In the IUPAC system:

- Removing a H from an alkane is called **alkyl group.**

-~~ane~~ $\longrightarrow$ **-yl**

- Halogen atoms are named as **halo**.

-~~ine~~ $\longrightarrow$ **-O**

Table 16.5 Names and Formulas of Some Common Substituents

Substituent	Name
$CH_3—$	methyl
$CH_3—CH_2—$	ethyl
$CH_3—CH_2—CH_2—$	propyl
F—, Cl—, Br—, I—	fluoro, chloro, bromo, iodo
-OH	Hydroxyl
$-NO_2$	Nitro

Give the name of:

$$\begin{array}{ccccccc} & & CH_3 & & & & \\ & & | & & & & \\ CH_3 & - & CH & - & CH_2 & - & CH_3 \end{array}$$

STEP 1 Longest chain is butane.

STEP 2 Number chain.

$$\begin{array}{ccccccc} & & CH_3 & & & & \\ & & | & & & & \\ CH_3 & - & CH & - & CH_2 & - & CH_3 \\ \mathbf{1} & & \mathbf{2} & & \mathbf{3} & & \mathbf{4} \end{array}$$

STEP 3 Locate substituents and name.

2-Methylbutane

$$\begin{array}{ccccc} & & Cl & CH_3 & \\ & & | & | & \\ \boxed{CH_3- & CH_2- & CH- & CH- & CH_3} \end{array}$$

STEP 1 Longest chain is pentane.

STEP 2 Number chain from end nearest substituent.

$$\begin{array}{ccccc} & Cl & CH_3 & & \\ & | & | & & \\ CH_3- & CH_2- & CH- & CH- & CH_3 \\ \mathbf{1} & \mathbf{2} & \mathbf{3} & \mathbf{4} & \mathbf{5} \end{array}$$

STEP 3 Locate substituents and name alphabetically.

2-Chloro-3-methylpentane

$$
\begin{array}{ccccccccc}
 & & CH_3 & & & & CH_3 & & \\
 & & | & & & & | & & \\
CH_3 & - & CH & - & CH_2 & - & CH & - & CH_3 \\
1 & & 2 & & 3 & & 4 & & 5
\end{array}
$$

2,4-dimethylpentane

$$
\begin{array}{ccccccccccccc}
 & & & & Cl & & & & CH_3 & & & & \\
 & & & & | & & & & | & & & & \\
CH_3 & - & CH_2 & - & CH & - & CH_2 & - & C & - & CH_2 & - & CH_3 \\
 & & & & & & & & | & & & & \\
 & & & & & & & & Cl & & & & \\
7 & & 6 & & 5 & & 4 & & 3 & & 2 & & 1
\end{array}
$$

3,5-dichloro-3-methylheptane

“classes of carbons”

primary carbon (1^o) – a carbon bonded to one carbon

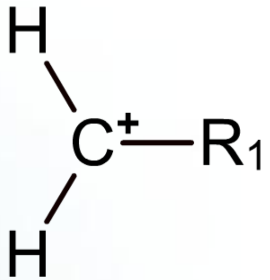
secondary carbon (2^o) – a carbon bonded to two carbons

tertiary carbon (3^o) – a carbon bonded to three carbons

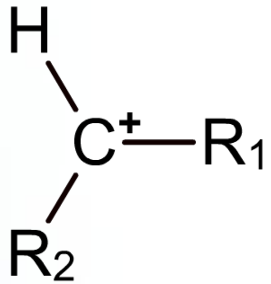
Structure of carbonations

A chain of carbon atoms can be represented by R when drawing organic structures. This is an **alkyl group** (general formula C_nH_{2n+1}).

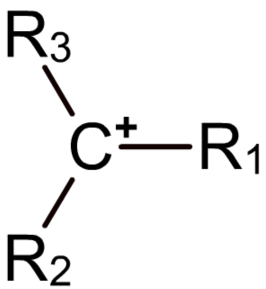
- **Primary (1°) carbonations** have one alkyl group attached to the positive-charged carbon.



- **Secondary (2°) carbonations** have two alkyl groups attached to the positive-charged carbon.

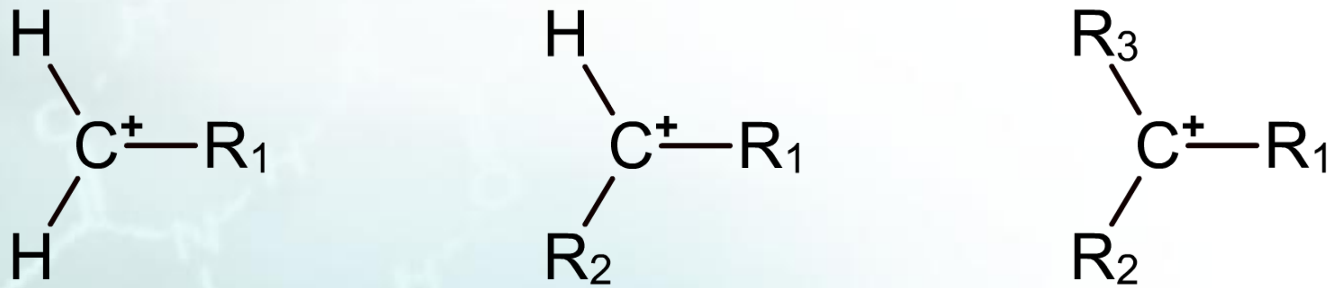


- **Tertiary (3°) carbonations** have three alkyl groups attached to the positive-charged carbon.



Stability of carbonations

The stability of carbonations increases as the number of alkyl groups on the positive-charged carbon atom increases.



primary **secondary** **tertiary**

increasing stability

The stability increases because alkyl groups contain a greater electron density than hydrogen atoms. This density is attracted towards, and reduces, the positive charge on the carbon atom, which has a stabilizing effect.

alkanes, physical properties

non-polar or only weakly polar, cannot hydrogen bond → relatively weak intermolecular forces

lower mp/bp; increase with size; decrease with branching

@ room temperature:

$C_1 – C_4$ are gases

$C_5 – C_{17}$ are liquids

$> C_{17}$ are solids

alkanes are water insoluble

Physical Properties of Alkanes

- Nonpolar
- Insoluble in water.
- Lower density than water.
- Low boiling and melting points.
- Gases with 1-4 carbon atoms.
- Liquids with 5-17 carbon atoms.
- Solids with 18 or more carbon atoms.

CH_4 (-161˚C) **C_2H_6 (-88˚C)** **C_3H_8 (-42˚C)** **C_4H_{10} (-0.5˚C)**

alkane	mp ^oC	bp ^oC
methane	-183	-162
ethane	-172	-89
propane	-187	-42
n-butane	-138	0
n-pentane	-130	36
n-hexane	-95	69
…		
n-heptadecane	22	292
n-octadecane	28	308

branching lowers mp/bp

n-pentane	-130	36
isopentane	-160	28

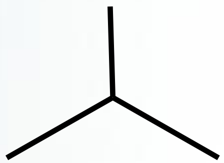
Boiling & melting points of Alkanes

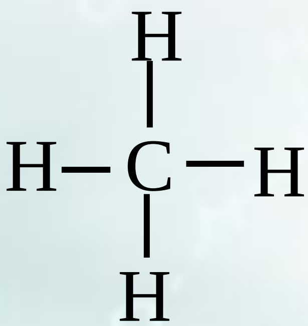
Number of carbon atoms ↑ $\Rightarrow$ bp & mp ↑

Number of branches ↑ $\Rightarrow$ bp & mp ↓

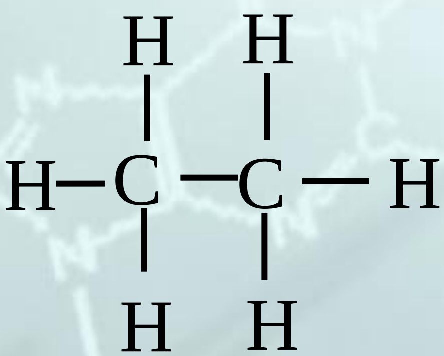
$CH_3CH_2CH_2CH_3$

$$\begin{array}{c} CH_3 \\ | \\ CH_3CHCH_3 \end{array}$$

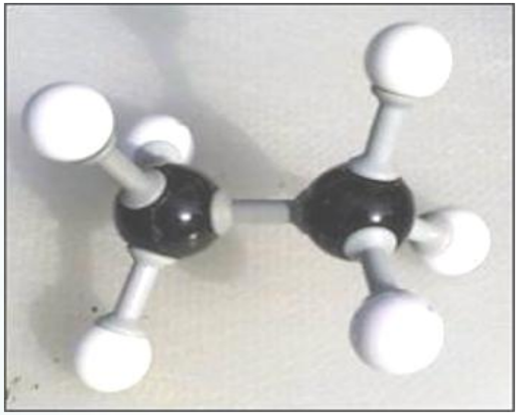


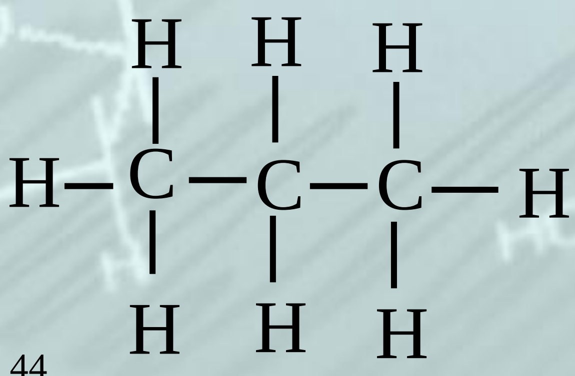


methane, CH_4

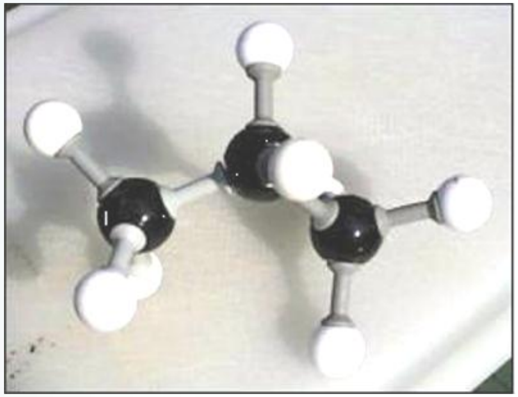


ethane, C_2H_6

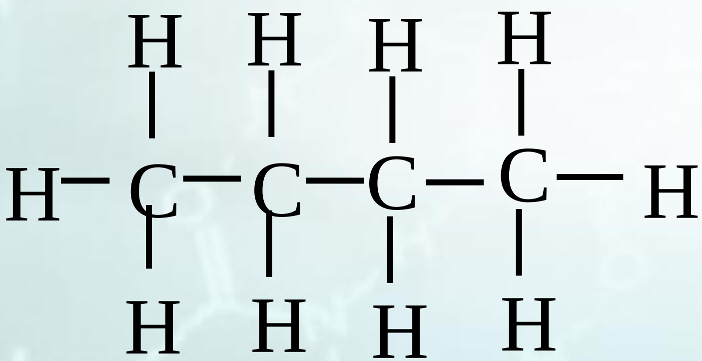


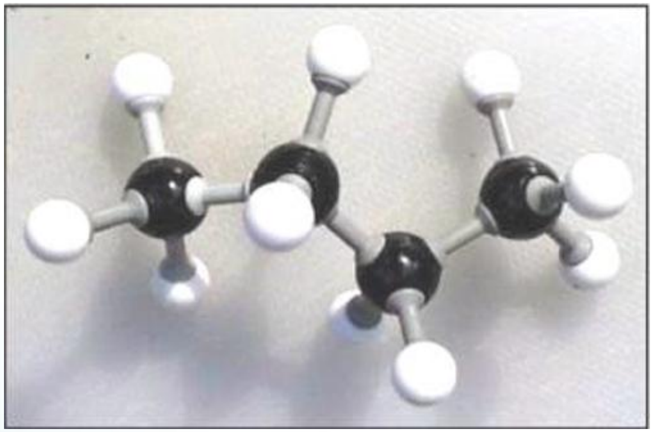


propane, C_3H_8

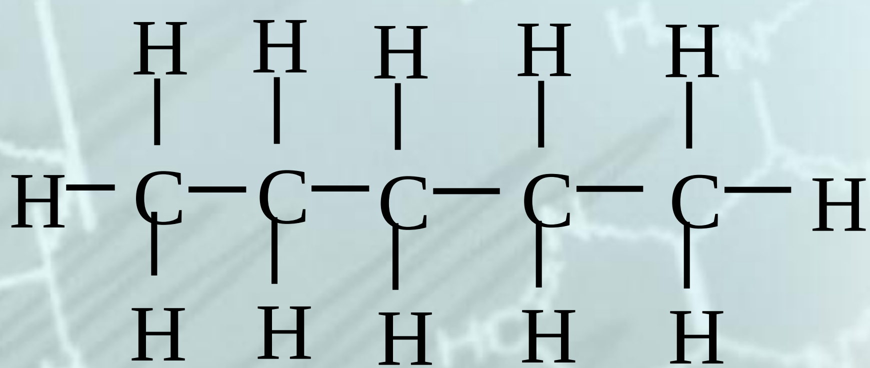


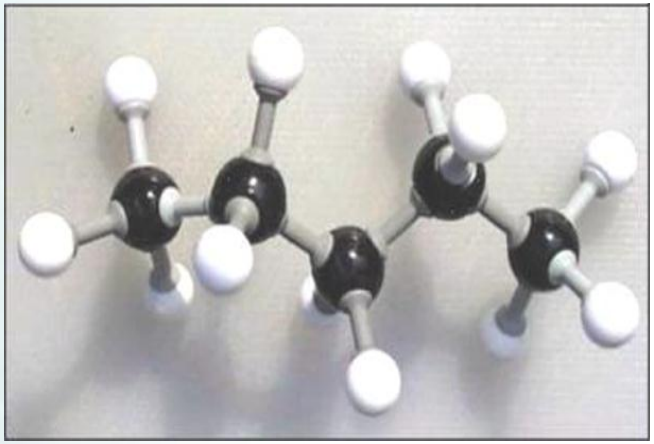
butane, C_4H_{10}



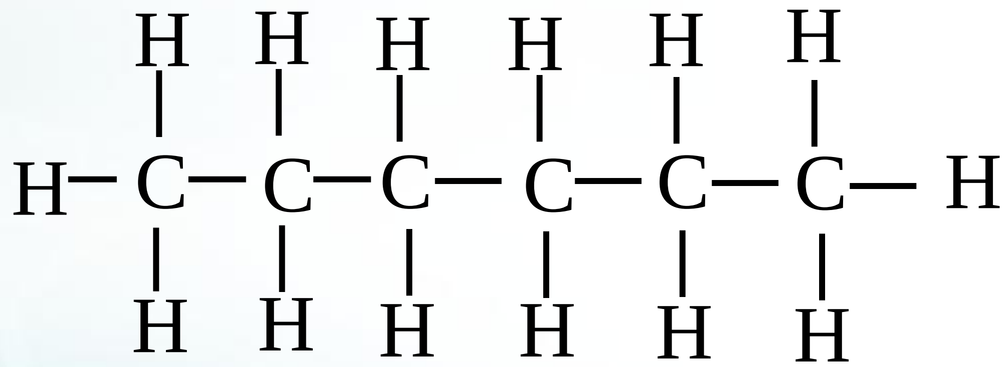


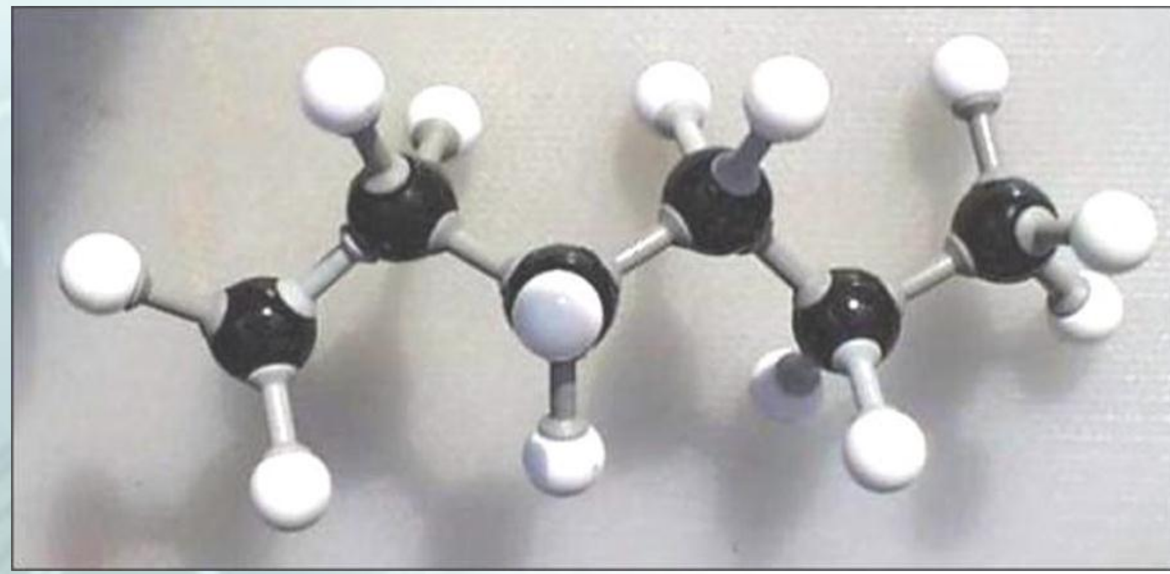
pentane, C_5H_{12}





hexane, C_6H_{14}





Alkanes, syntheses

Reduction of an alkyl halide

a) hydrolysis of a Grignard reagent (two steps)

i) R—X + Mg → RMgX (Grignard reagent)

ii) RMgX + H_2O → RH + Mg(OH)X

SB SA WA WB

$CH_3CH_2CH_2$-Br + Mg → $CH_3CH_2CH_2$-MgBr

n-propyl bromide *n*-propyl magnesium bromide

$CH_3CH_2CH_2$-MgBr + H_2O → $CH_3CH_2CH_3$ + Mg(OH)Br

propane

Reactions of alkanes:

alkane + H_2SO_4 → no reaction (NR)

alkane + NaOH → NR

alkane + Na → NR

alkane + $KMnO_4$ → NR

alkane + H_2,Ni → NR

alkane + Br_2 → NR

alkane + H_2O → NR

(Alkanes are typically non-reactive. They don't react with acids, bases, active metals, oxidizing agents, reducing agents, halogens, etc.)

$$CH_3CH_3 \quad + \quad Cl_2, hv \quad \rightarrow \quad CH_3CH_2\text{-}Cl \quad + \quad HCl$$

ethane — ethyl chloride

$$CH_3CH_2CH_3 \quad + \quad Cl_2, hv \quad \rightarrow \quad CH_3CH_2CH_2\text{-}Cl \quad + \quad \underset{\displaystyle Cl}{CH_3CHCH_3}$$

propane — *n*-propyl chloride — isopropyl chloride

45% — 55%

gives a mixture of both the possible alkyl halides! ☹

CH_3CH_3 + Cl_2, hv → CH_3CH_2-Cl + HCl

ethane — ethyl chloride

$CH_3CH_2CH_3$ + Cl_2, hv → $CH_3CH_2CH_2$-Cl + CH_3CHCH_3 (Cl)

propane — *n*-propyl chloride (45%) — isopropyl chloride (55%)

gives a mixture of both the possible alkyl halides! ☹

b) with an active metal and an acid

R—X + metal/acid → RH

active metals = Sn, Zn, Fe, etc.

acid = HCl, etc. (H^+)

$$\underset{\displaystyle Cl\quad}{CH_3CH_2CHCH_3} \quad + \quad Sn/HCl \quad \rightarrow \quad CH_3CH_2CH_2CH_3 \quad + \quad SnCl_2$$

sec-butyl chloride *n*-butane

$$\overset{\displaystyle CH_3}{\underset{\displaystyle Br}{CH_3CCH_3}} \quad + \quad Zn/H^+ \quad \rightarrow \quad \overset{\displaystyle CH_3}{CH_3CHCH_3} \quad + \quad ZnBr_2$$

tert-butyl bromide isobutane

Cycloalkanes

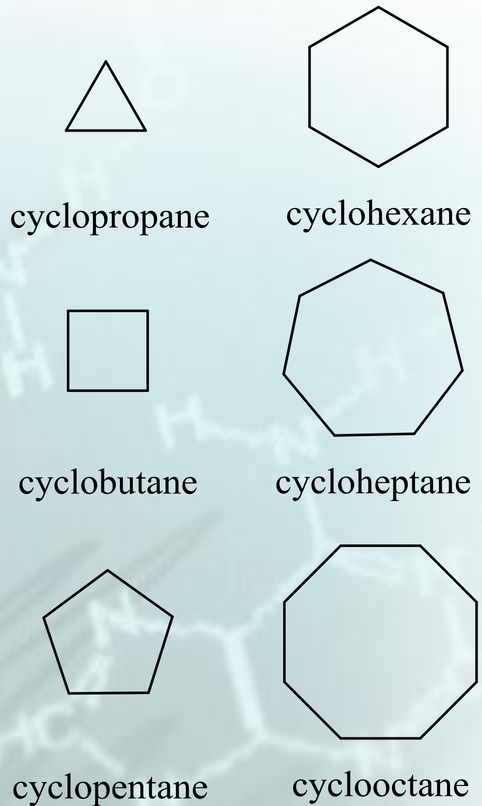
Cycloalkanes

An import out and inder setting group of hydrocarbon, contain ring of carbon atoms.

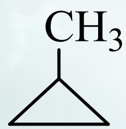
Linked together by single bound the general formula of cycle alkanes is C_nH_{2n}

Naming of cycloalkanes

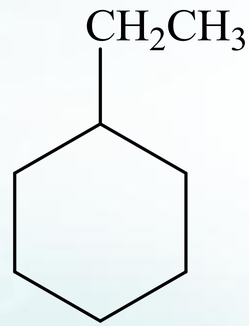
Cycloalkanes is named by adding prefix cyclo to the corresponding n-alkanes



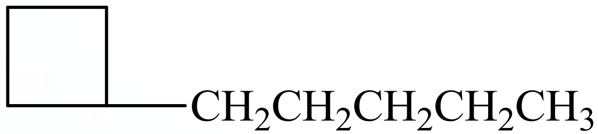
Substituted cycloalkanes are name by cycloalkane.



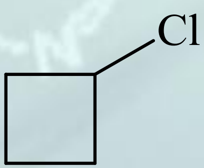
Methylcyclopropane



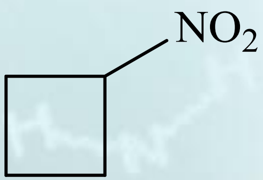
Ethylcyclohexane



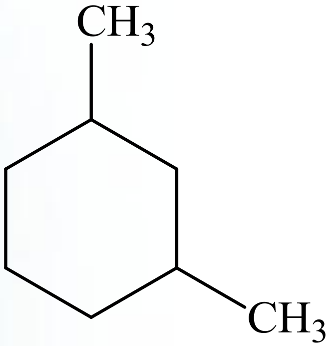
1-cyclobutylpentane



Chlorocyclobutane



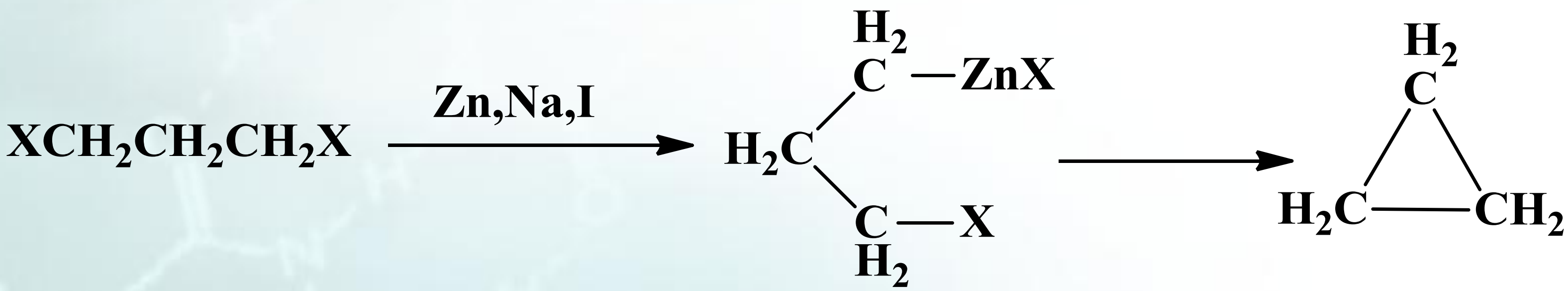
Nitrocyclobutane



1,3-dimethylcyclohexane

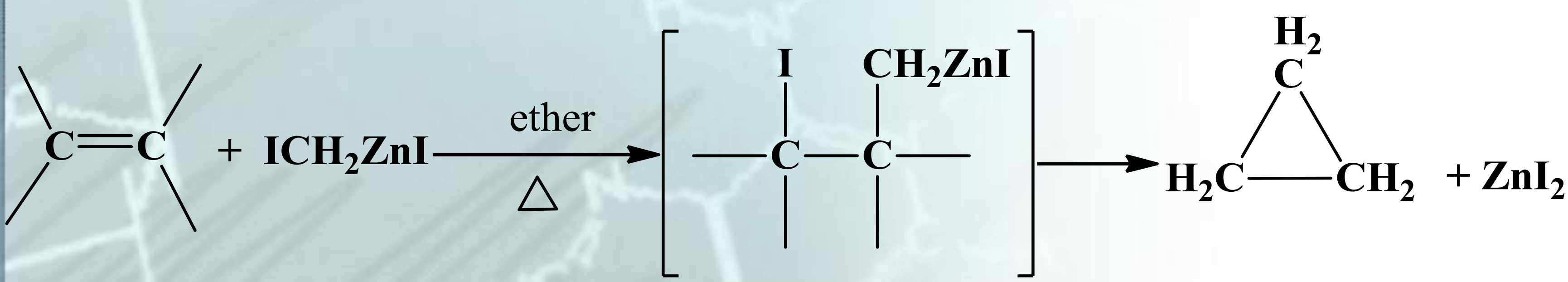
Preparation of cyclopropane

1- by wurts reaction



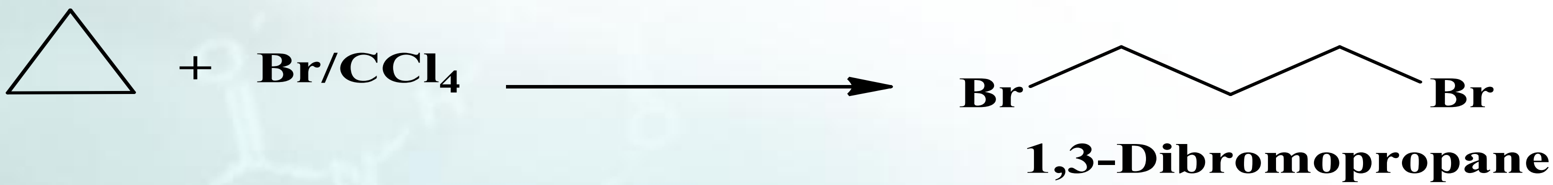
2-Suaon-Smith reaction

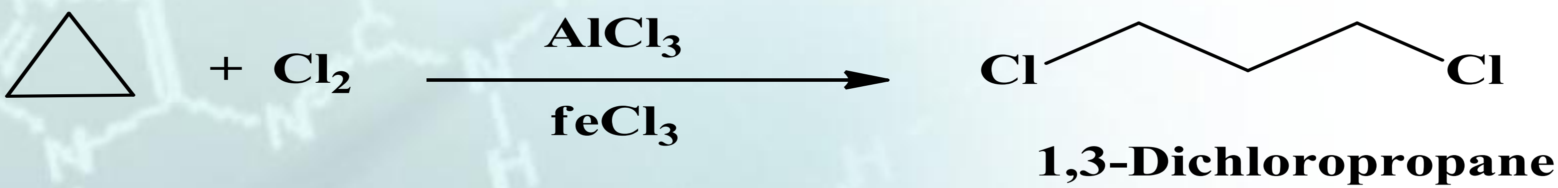
$$CH_2I_2 + Zn(Cu) \longrightarrow ICH_2ZnI$$



Reactions of Cyclopropane

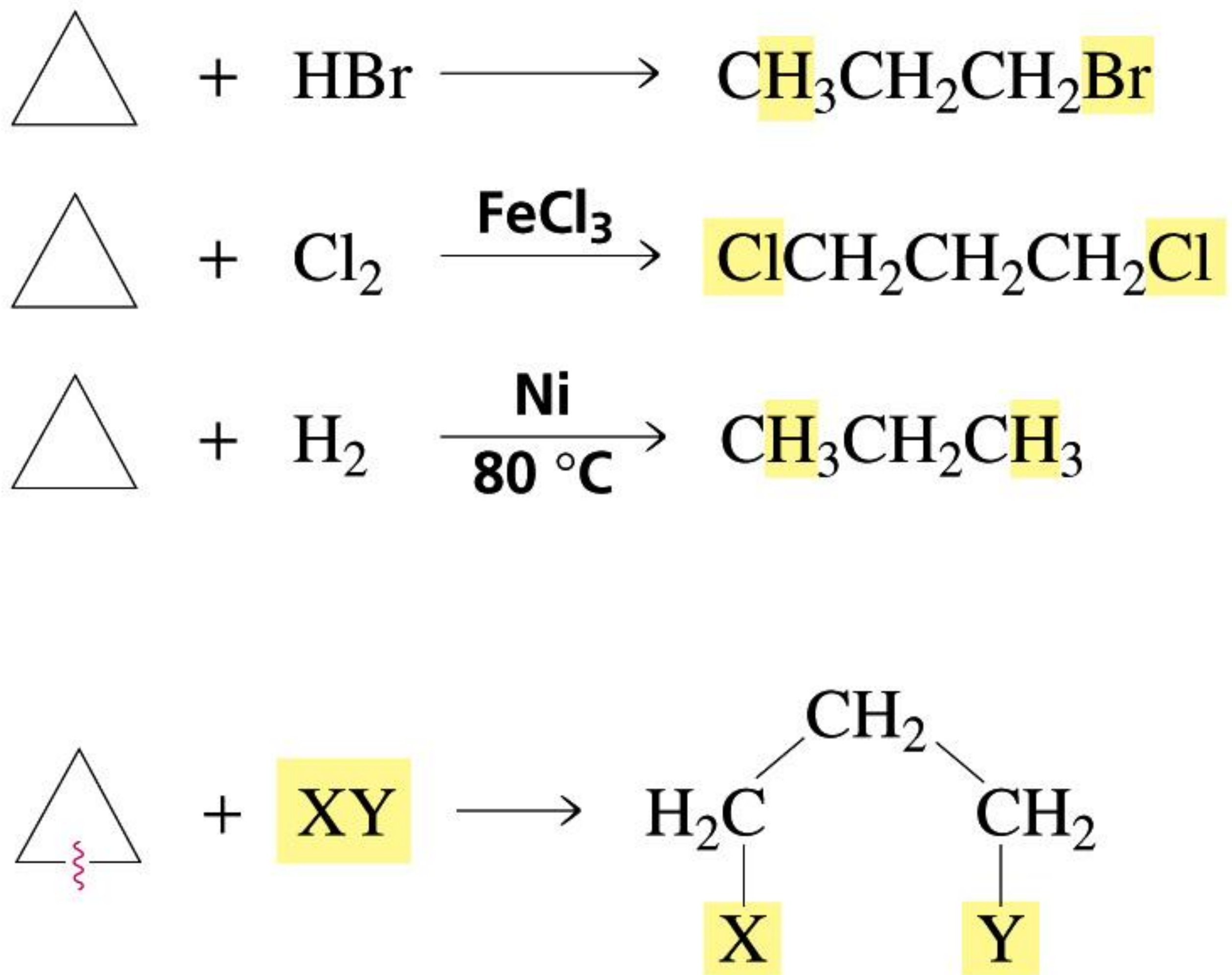
1-addition of hydrogen.



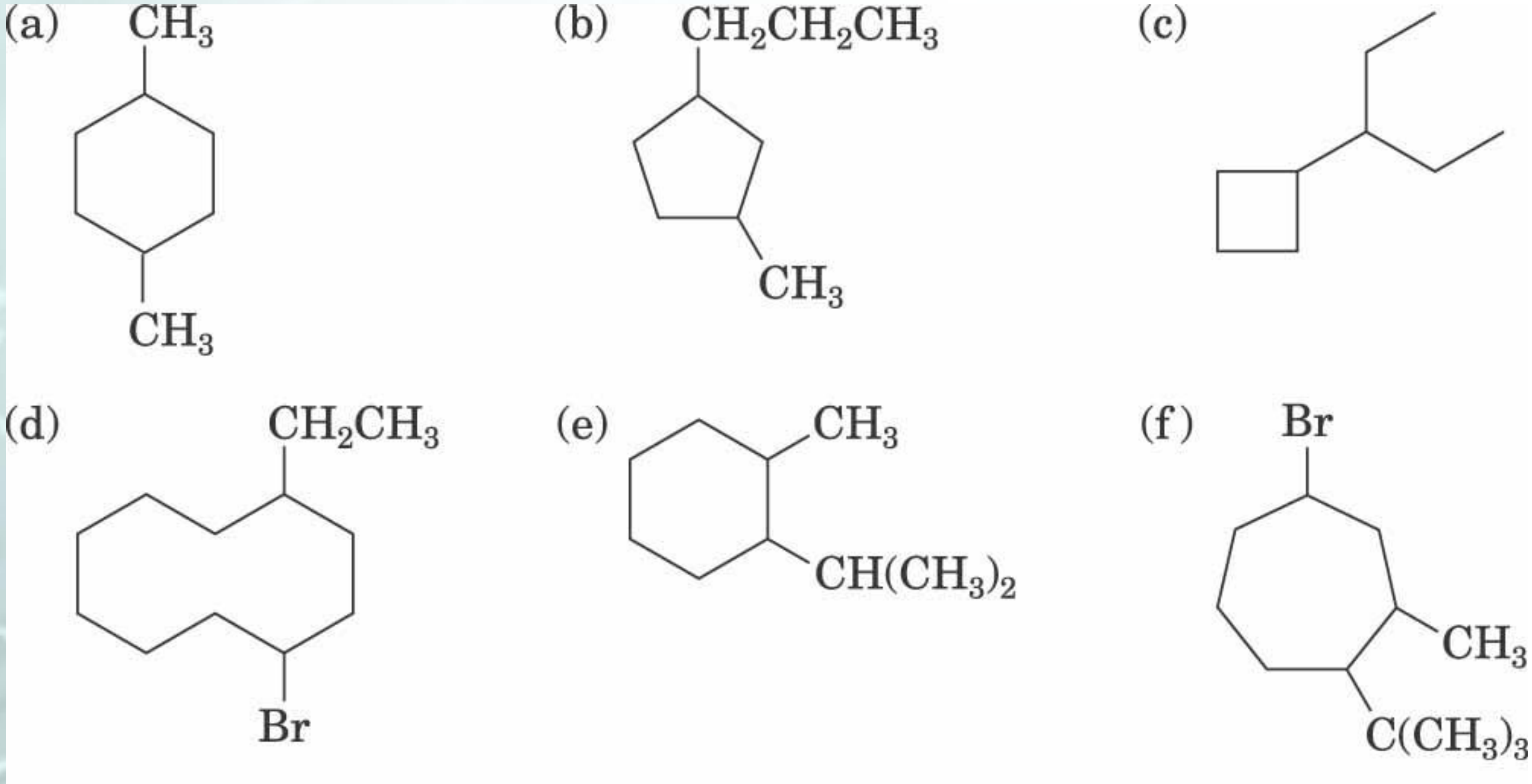


2-addition of H_2SO_4

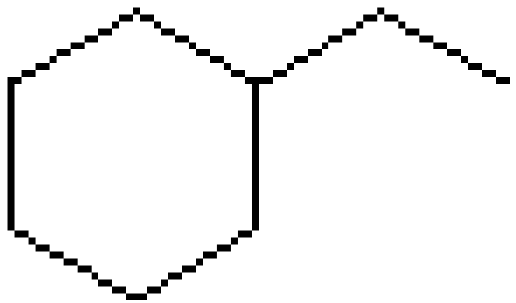
Reactions of Cyclopropane



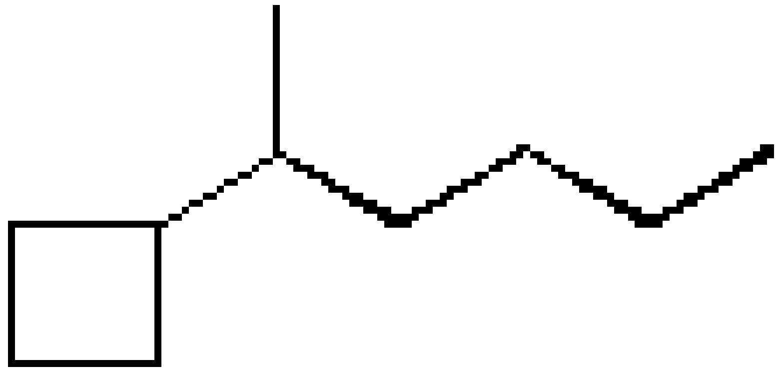
IUPAC names



(a)
CH_3
CH_3
(b)
$CH_2CH_2CH_3$
CH_3
(c)
(d)
CH_2CH_3
Br
(e)
CH_3
$CH(CH_3)_2$
(f)
Br
CH_3
$C(CH_3)_3$



ethylcyclohexane



2-cyclobutylhexane

Which of these is an alkane?

A. C_6H_{14}

B. C_4H_8

C. $C_{12}H_{24}$

D. $C_{102}H_{204}$

Thank You