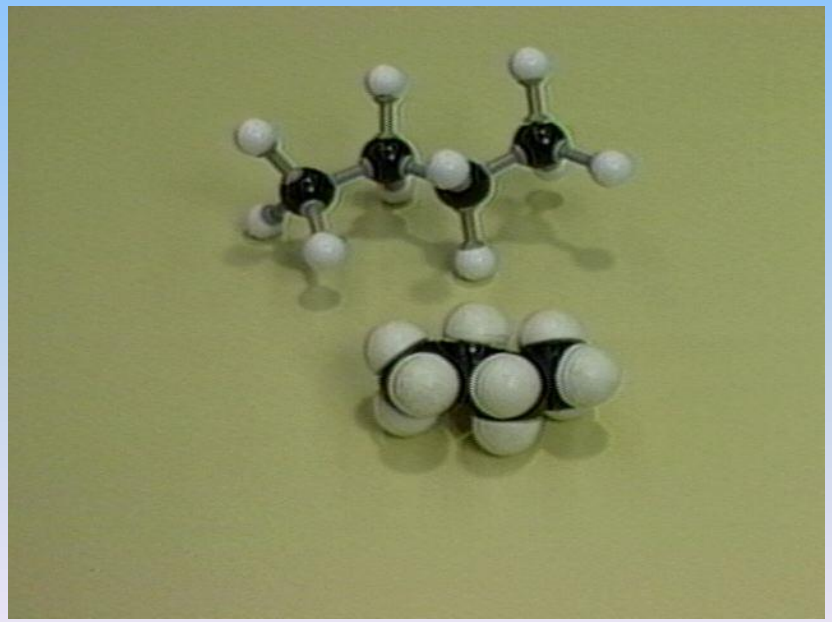
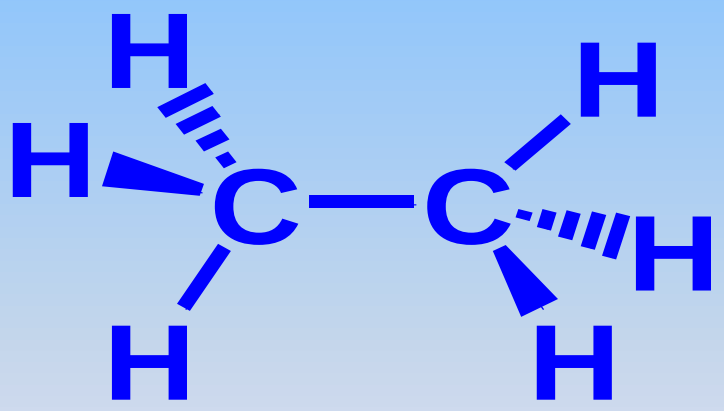
Chapter (2)

Alkanes (Paraffines) and Cycloalkanes





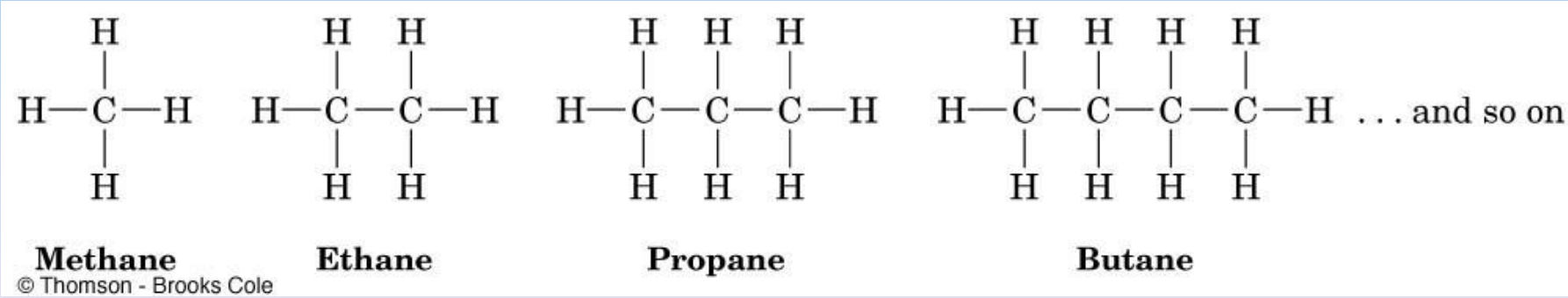
Ethane

Alkanes and Alkane Isomers

- **Alkanes are saturated aliphatic compounds**

(Contains only C and H)

- **Alkanes contain only sp^3 hybridized Carbon**
- **Alkanes have only single C—C single bonds and C-H bonds only.** (no functional groups).
- **Alkane have a general formula (law) of C_nH_{2n+2}**
- Connecting carbons can lead to **large or small molecules.**

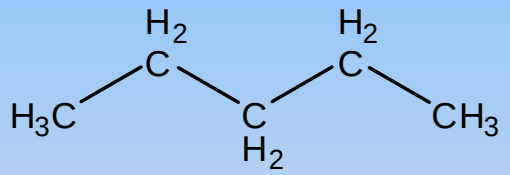


the First Ten Continuous-Chain Alkanes

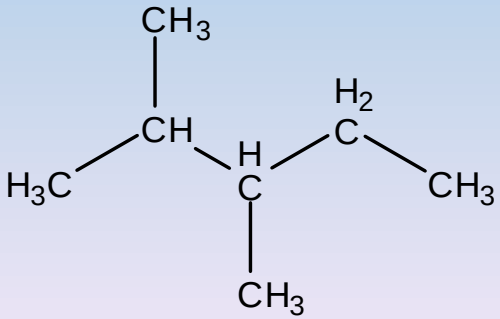
Alkane	Formula C_nH_{2n+2}
• Methane	CH_4
• Ethane	CH_3CH_3
• Propane	$CH_3CH_2CH_3$
• Butane	$CH_3(CH_2)_2CH_3$
• Pentane	$CH_3(CH_2)_3CH_3$
• Hexane	$CH_3(CH_2)_4CH_3$
• Heptane	$CH_3(CH_2)_5CH_3$
• Octane	$CH_3(CH_2)_6CH_3$
• Nonane	$CH_3(CH_2)_7CH_3$
• Decane	$CH_3(CH_2)_8CH_3$

Alkane Isomers

- Alkanes with C's connected to no more than 2 other C's are **straight-chain (normal) alkanes (n).**
- Alkanes with one or more C's connected to 3 or 4 C's are **branched-chain alkanes.**



straight-chain



branched-chain

Hybridization of Alkanes

$C(6) - 1s^2, 2s^2, 2p_x^1, 2p_y^1, 2p_z^0$

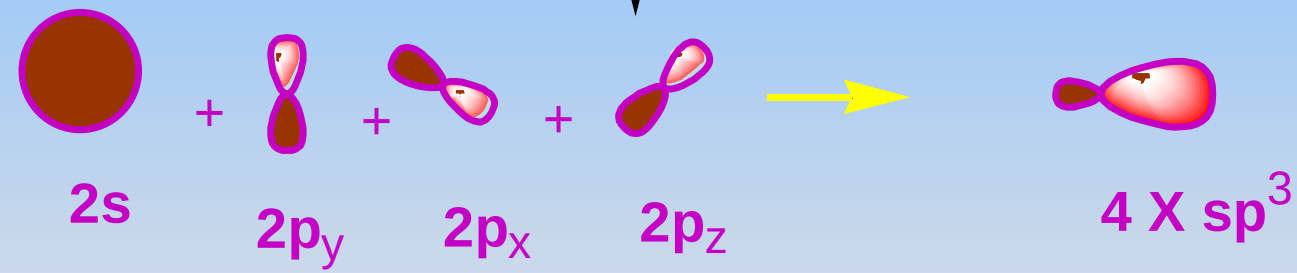
lowest energy state

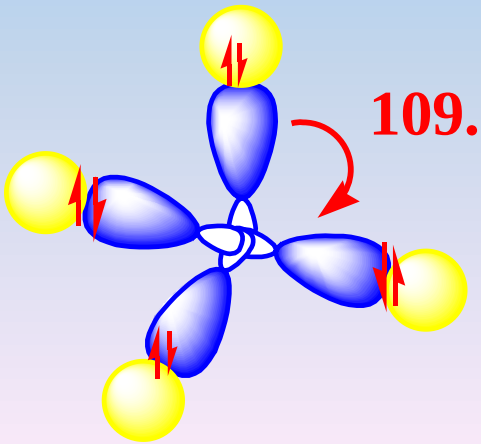
$C(6) - 1s^2, 2s^1, 2p_x^1, 2p_y^1, 2p_z^1$

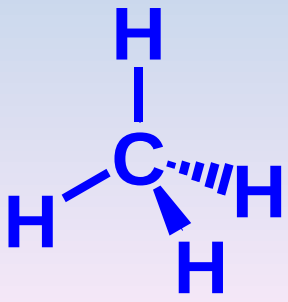
Excited state

Methane is Tetrahedral

4 sp^3 *Hybridization*

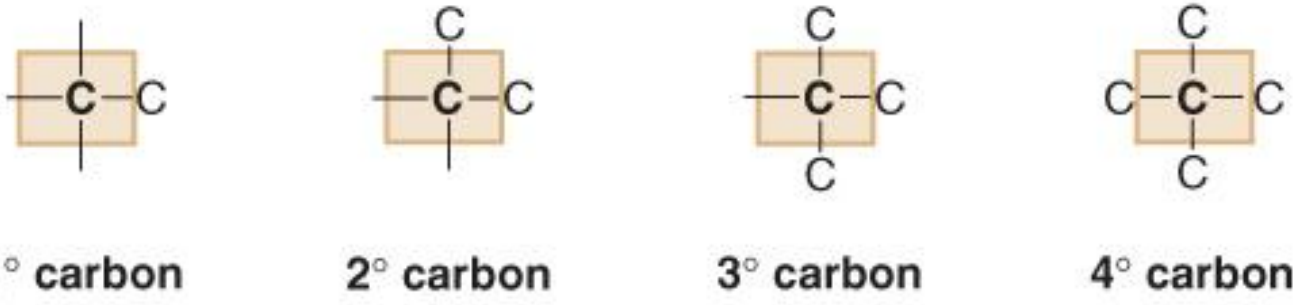




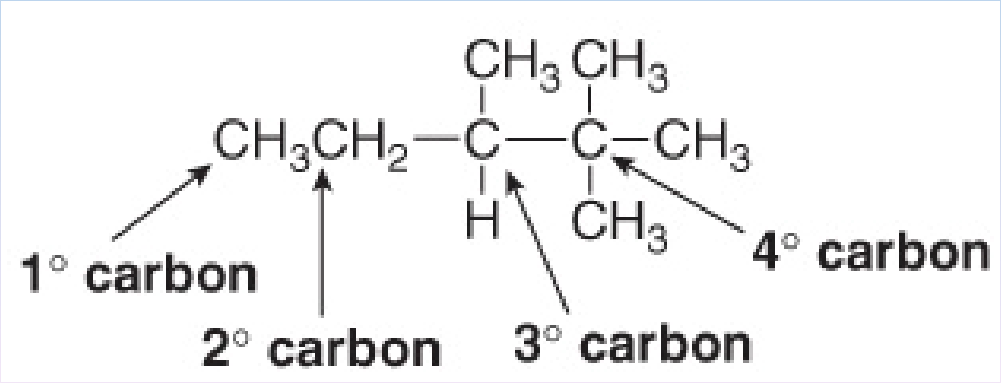


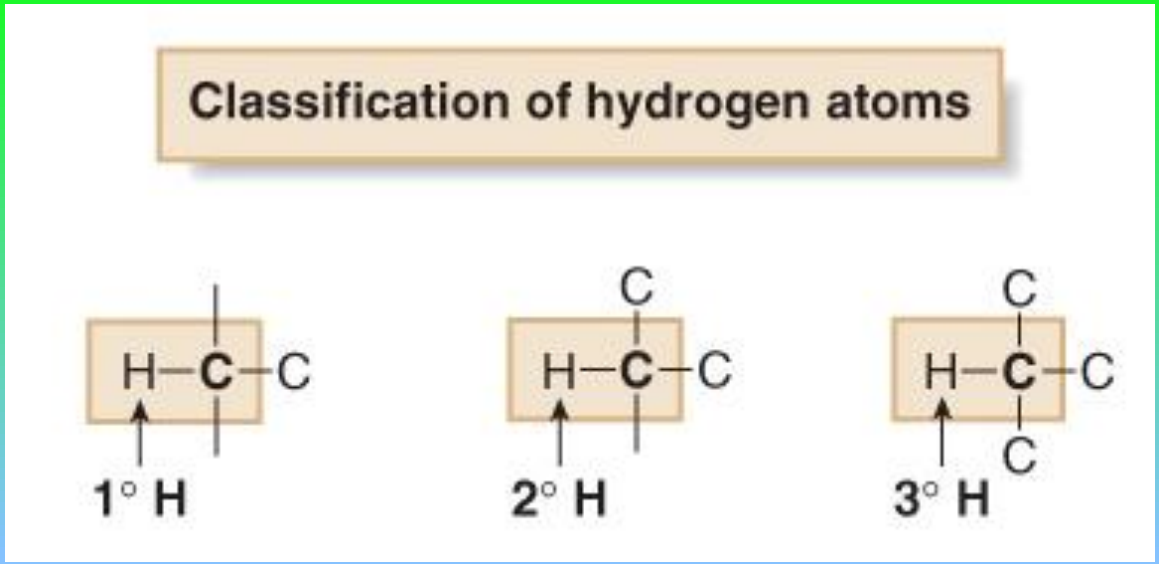
Sp³ hybridized carbon
4 equivalent C-H bonds (σ–bonds)
All purely single bonds are called σ–bonds

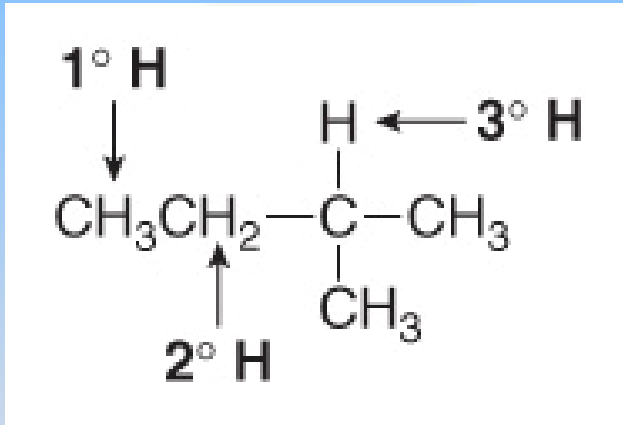
Classification of carbon atoms



- A *primary carbon* (1° carbon) is bonded to *one* other C atom.
- A *secondary carbon* (2° carbon) is bonded to *two* other C atoms.
- A *tertiary carbon* (3° carbon) is bonded to *three* other C atoms.
- A *quaternary carbon* (4° carbon) is bonded to *four* other C atoms.







- Hydrogen atoms are classified as primary (1°), secondary (2°), or tertiary (3°) depending on the type of carbon atom to which they are bonded.

Alkyl groups (R)

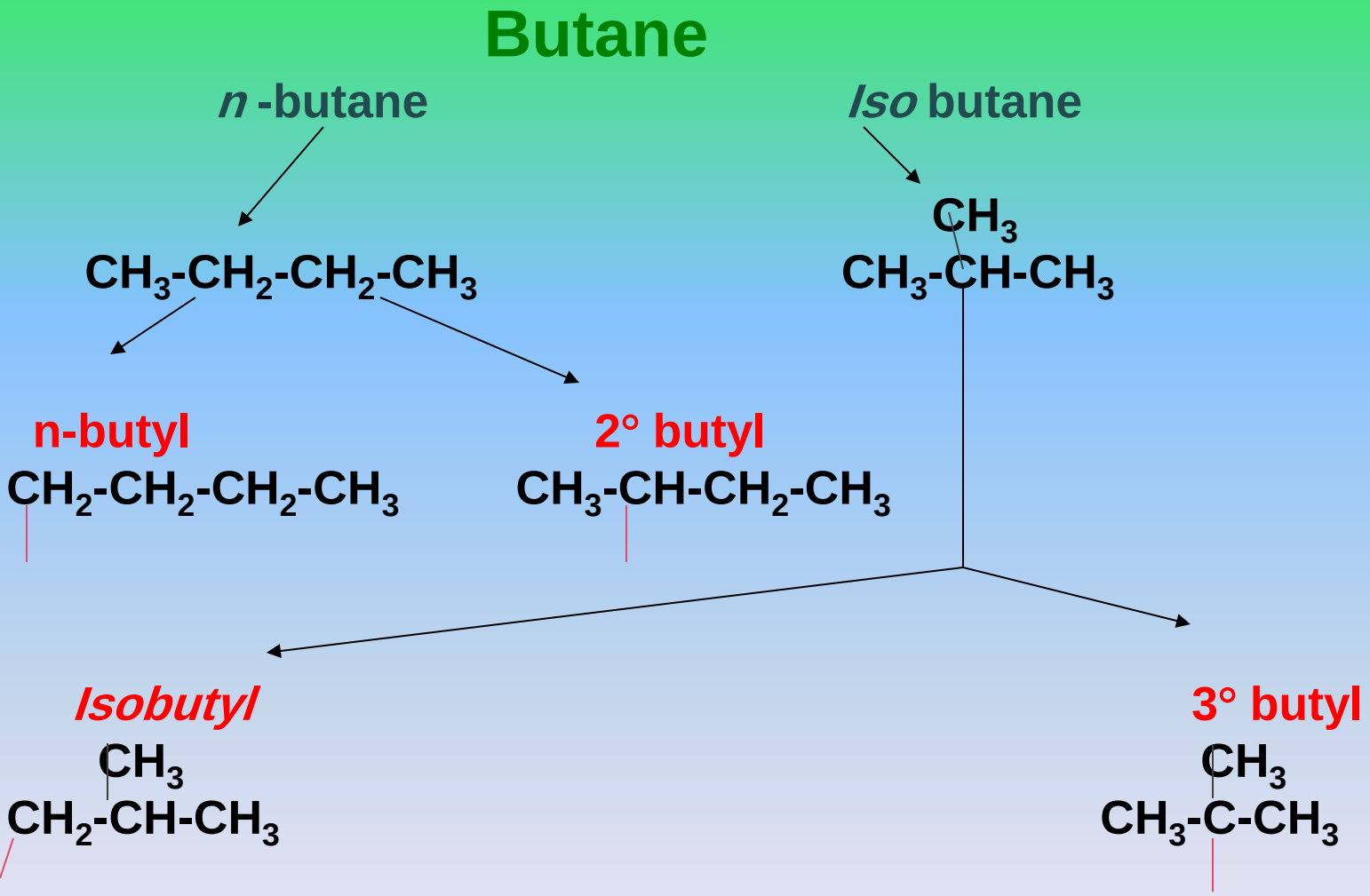
R- H ---------- R-
- H

Alkane — Alkyl group

- **Methane** CH_4 CH_3 **Methyl**
- **Ethane** C_2H_6 C_2H_5 **Ethyl**

- **Propane** C_3H_8 **(2 R)**
- $CH_3\text{-}CH_2\text{-}CH_3$
- $\text{-}\ CH_2\text{-}CH_2\text{-}CH_3$ **OR** $CH_3\text{-}CH\text{-}CH_3$
- **n-Propyl** **Isopropyl**

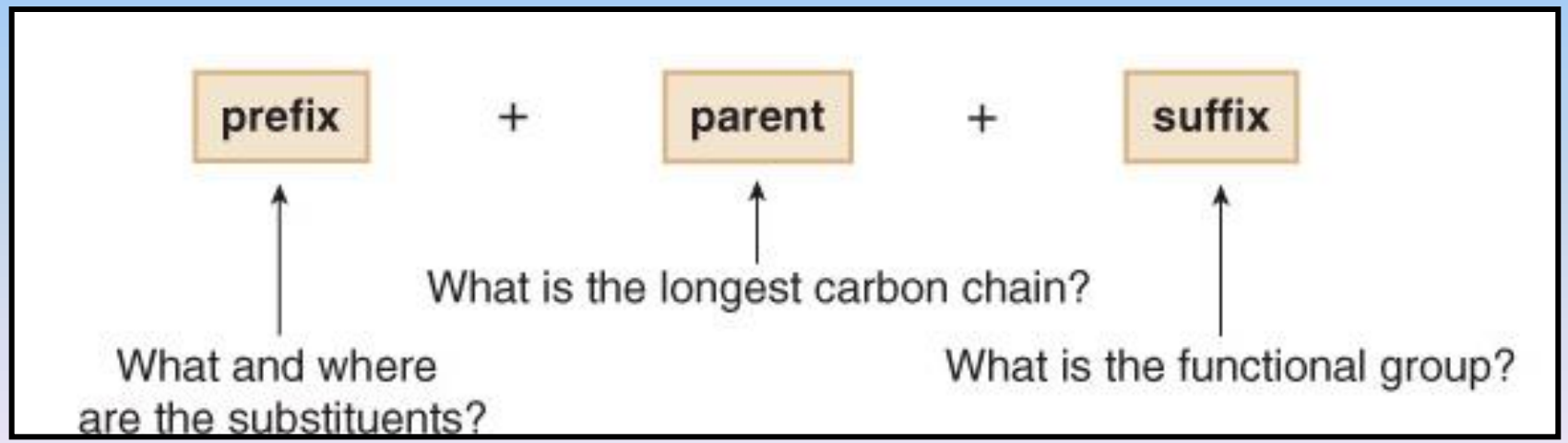
Butane (C_4H_{10})



IUPAC Nomenclature

The name of every organic molecule has **3** parts:

1. The ***parent name*** indicates the number of carbons in the longest continuous chain.
2. The ***suffix*** indicates what functional group is present.
3. The ***prefix*** tells us the identity, location, and number of substituents attached to the carbon chain.



Naming Alkanes

- **Follows specific rules**
- **Find the <u>longest continuous</u> (parent carbon) chain and add the suffix.**
- **If there are two chains of <u>equal length</u>, pick the chain with more substituents.**
- **Number the atoms in the carbon chain to give the first substituent the lowest number.**
- **When numbering a carbon chain results in the same numbers from either end of the chain, assign the lower number alphabetically to the first substituent.**
- **Use prefixes *di-, tri-, tetra-*, when there is more than one alkyl branch of the same kind.**

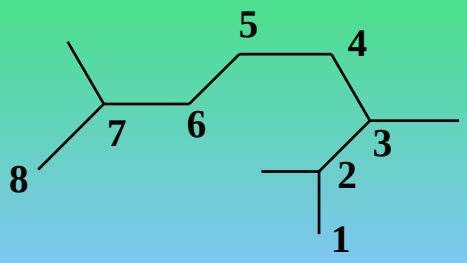
Recall:

1. Comma (,) separate numbers only: 2,3, ...

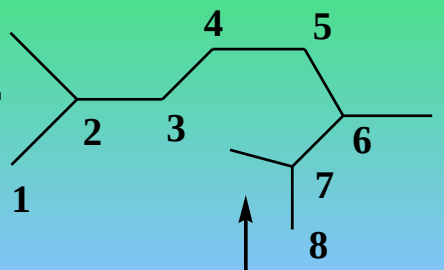
2. dash (-) separate numbers from names: 2-methyl.....

Examples

1



NOT



1. Parent compound has 8 carbons ⟶ Octane

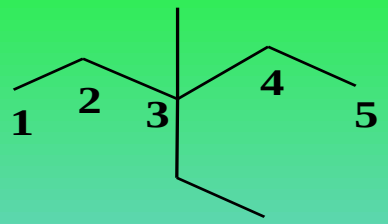
2. Substituents:

group	Name	location
CH_3	methyl	2
CH_3	methyl	3
CH_3	methyl	7

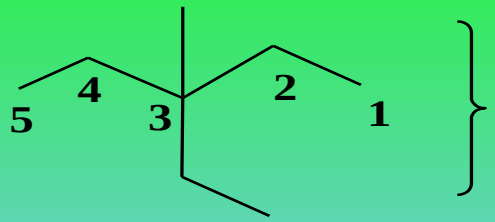
2,3,7-Trimethyloctane NOT 2,6,7-Trimethyloctane

Its wrong to say 2-methyl-3-methyl-7-methyloctane

2



OR



The Same
Why?

1. Parent compound has 5 carbons ⟶ Pentane

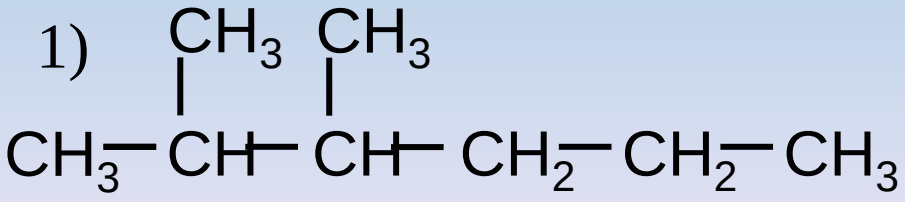
2. Substituents:

group	Name	location
CH_3	methyl	3
CH_2CH_3	ethyl	3

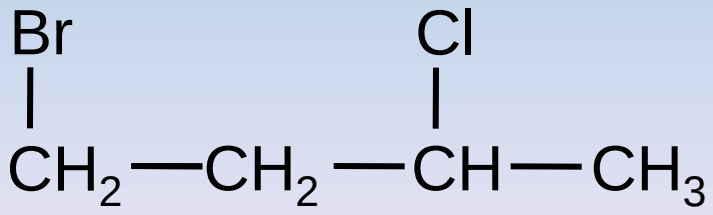
Ethyl is listed befor methyl for alphabetizing purposes

3-Ethyl-3-methylpentane

1)

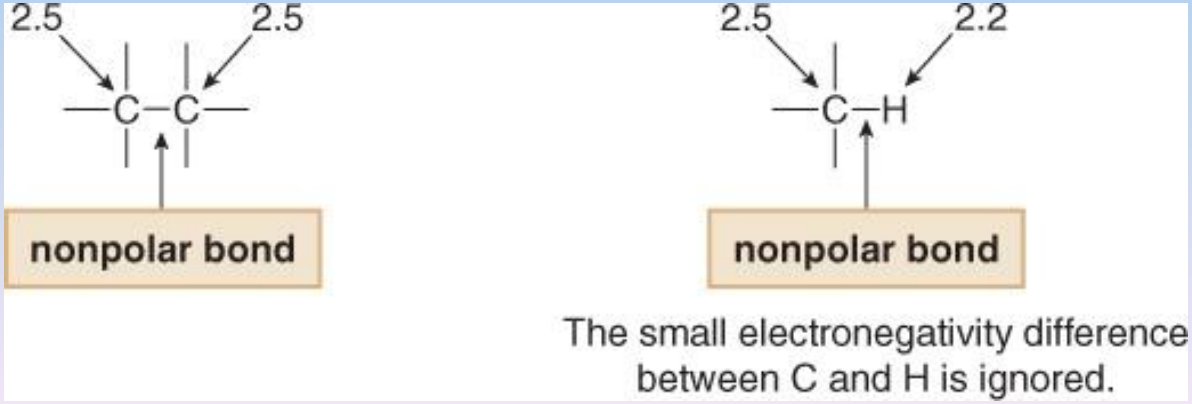


2)



Properties of Alkanes

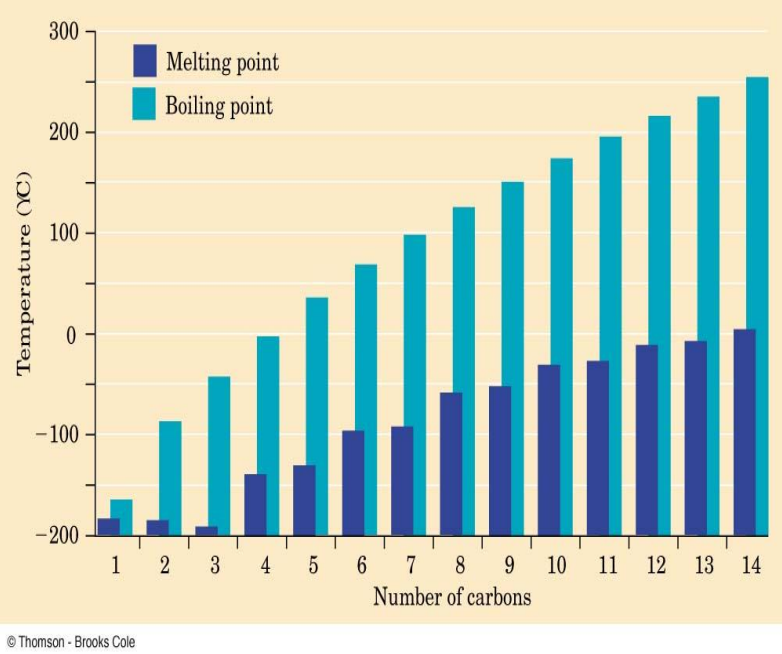
- Called **paraffins** (low affinity compounds) because they do not react as most chemicals
- They will burn in a flame, producing carbon dioxide, water, and heat
- ***Solubility in water***: Alkanes are insoluble in H_2O why?

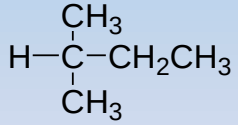
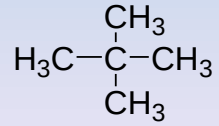


Alkanes are non-Polar compound

Physical Properties

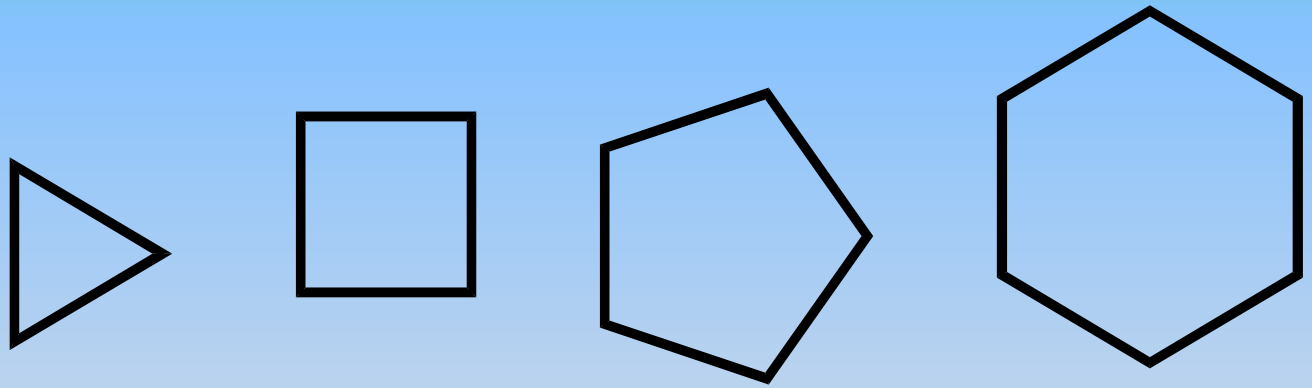
- Boiling points and melting points increase as size of alkane increases for straight chain alkanes, However, as branching increases, boiling point decreases
- Forces between molecules (temporary dipoles, dispersion) are weak



IUPAC name	Formula	Boiling point (B.P)
Pentane	$CH_3(CH_2)_3CH_3$	36
2-methylbutane		28
2,2-dimethylpropane		10

Cycloalkanes

- **Cycloalkanes** are alkanes that have carbon atoms that form a ring (called alicyclic compounds)
- Simple cycloalkanes rings of —CH_2— units, $(CH_2)_n$, or C_nH_{2n}
- Structure is shown as a regular polygon with the number of vertices equal to the number of C's (a projection of the actual structure)



Cyclopropane

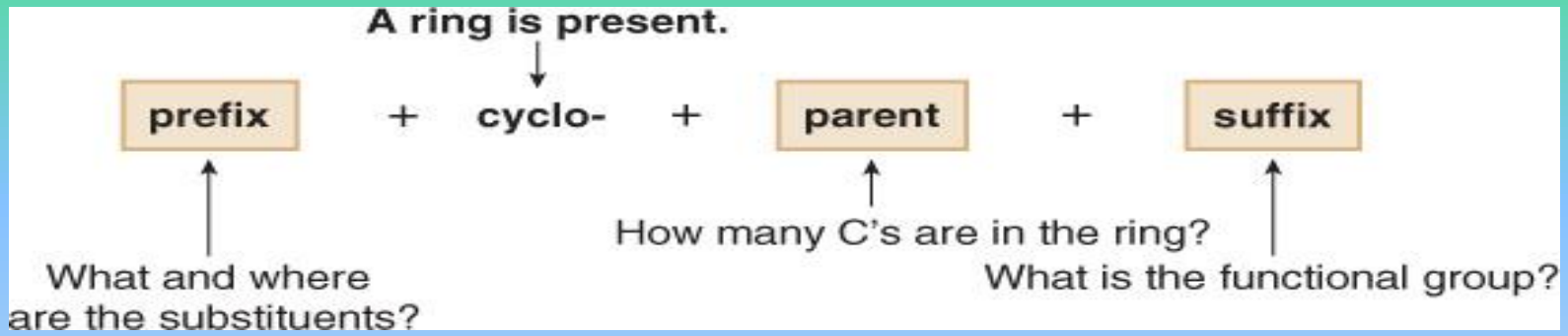
Cyclobutane

Cyclopentane

Cyclohexane

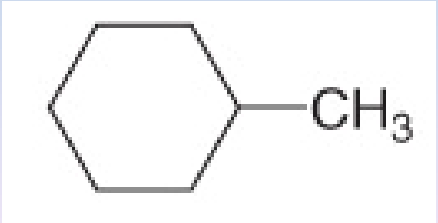
Nomenclature

Cycloalkanes are named by using similar rules, but the prefix cyclo- immediately precedes the name of the parent.



Find the parent cycloalkane.

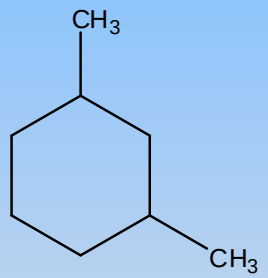
For Monosubstituted cycloalkanes, No number is needed to indicate the location of a single substituent.



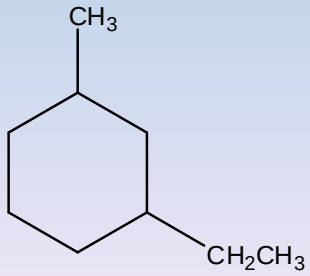
Methylcyclohexane

For disubstituted cycloalkanes

1. For rings with more than one substituent, begin numbering at one substituent and proceed around the ring to give the second substituent the lowest number.
2. **With two different substituents, number the ring to assign the lower number to the substituents alphabetically**.



1,3-Dimethylcyclohexane



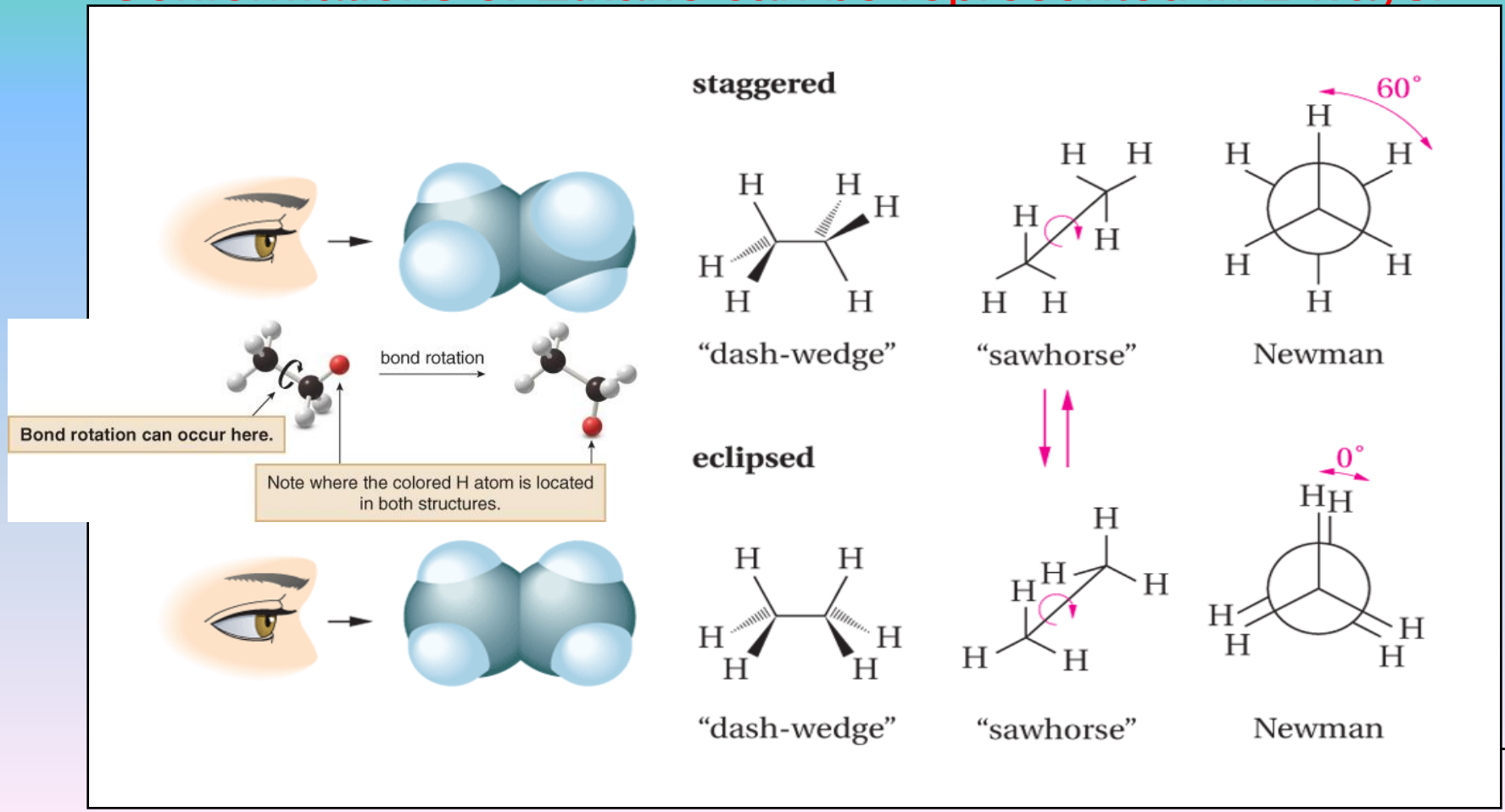
1-Ethyl-3-methylcyclohexane

Conformation Analysis of Alkane

Conformation:

Different arrangement of atoms resulting from bond free rotation around C-C single (σ) bond

Conformations of Ethane can be represented in 2 ways:



- There is a barrier to rotation, and some conformers are more stable than others
- **Staggered**- most stable: all 6 C-H bonds are as far away as possible
- **Eclipsed**- least stable: all 6 C-H bonds are as close as possible to each other

Reactions of Alkanes

1. Combustion(Oxidation) of Alkanes:

(Complete Combustion)

C_nH_{2n+2} + $(3n+1)/2\ O_2$ ⟶ $n\ CO_2$ + $(n+1)\ H_2O$ + heat

Alkane — Oxygen — Carbon dioxide — Water

Exothermic reaction

$CH_4 + 2\ O_2 \longrightarrow CO_2 + 2\ H_2O$ + heat

$CH_3\text{-}CH_2\text{-}CH_3 + 5\ O_2 \longrightarrow 3\ CO_2 + 4\ H_2O$ + heat

Two points concerning this reaction are important:

1. Since all the covalent bonds in the reactant molecules are broken, the quantity of heat evolved in this reaction is related to the strength of these bonds (and, of course, the strength of the bonds formed in the products).

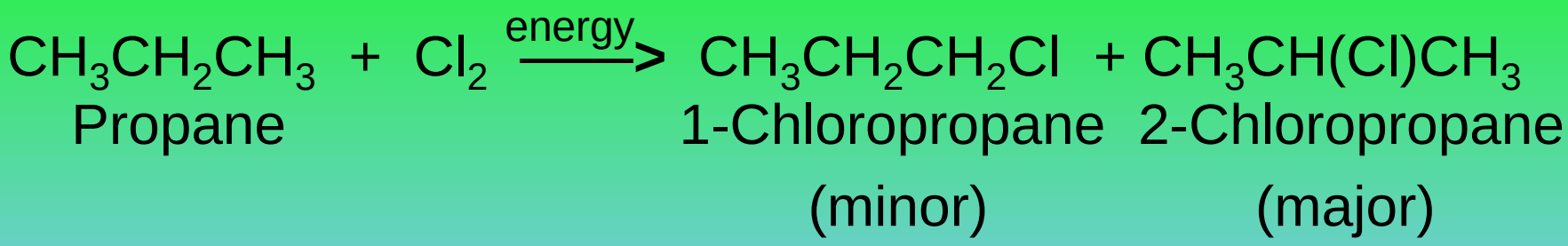
2. The stoichiometry of the reactants is important.

- **2. Halogenation:**
- Halogenation is the replacement (substitution) of one or more hydrogen atoms in saturated hydrocarbons by a halogen (Cl_2 or Br_2) in presence of energy (Heat or Light).

$$\underset{\text{Alkane}}{R\text{-}H} + \underset{\text{Halogen}}{X_2\ (Cl_2 \text{ or } Br_2)} \xrightarrow{\text{energy}} \underset{\text{Haloalkane}}{R\text{--}X} + H\text{-}X$$

- $CH_4 + Cl_2 \xrightarrow{\text{Heat}} CH_3Cl + HCl$

  Methane — Chloromethane
- one complication is that all the hydrogen atoms of an alkane may undergo substitution, resulting in a mixture of products
- $CH_4 + Cl_2 \xrightarrow{\text{Heat}} CH_3Cl + CH_2Cl_2 + CHCl_3 + CCl_4 + HCl$



Reactivity of Halogens towards halogenation of Alkanes:

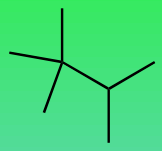
$$F_2 > Cl_2 > Br_2 > I_2$$

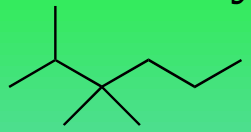
Reactivity of Hydrogens towards halogenation of Alkanes:

$$3^o > 2^o > 1^o$$

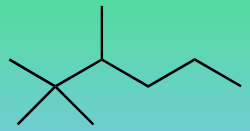
Practice Problems

1. The structural formula for 2,2,3-trimethylhexane is

a. 

b. 

c. $(CH_3)_2CCH_2CH_3$ with CH_3 below

***d.** 

e. $(CH_3)_3CCHCH_3$ with CH_3 below

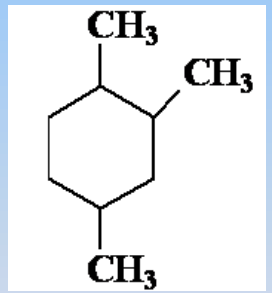
2. What is the molecular formula of a cycloalkane that has five carbon atoms?

***a.** C_5H_{10} **b.** C_5H_{12} **c.** C_5H_{14} **d.** C_5H_8

3. The IUPAC name is

a. 1,2,4-trimethylhexane *b. 1,2,4-trimethylcyclohexane

c. 1,3,4-trimethylcyclohexane d. 1,2,4-methylcyclohexane



4. Which of the following alkanes would have the highest boiling point?

a.pentane b.isopentane c.neopentane *d.hexane

THE END OF CHAPTER 2
ALKANES AND CYCLOALKANES

BEST WISHES AND GOOD LUCK