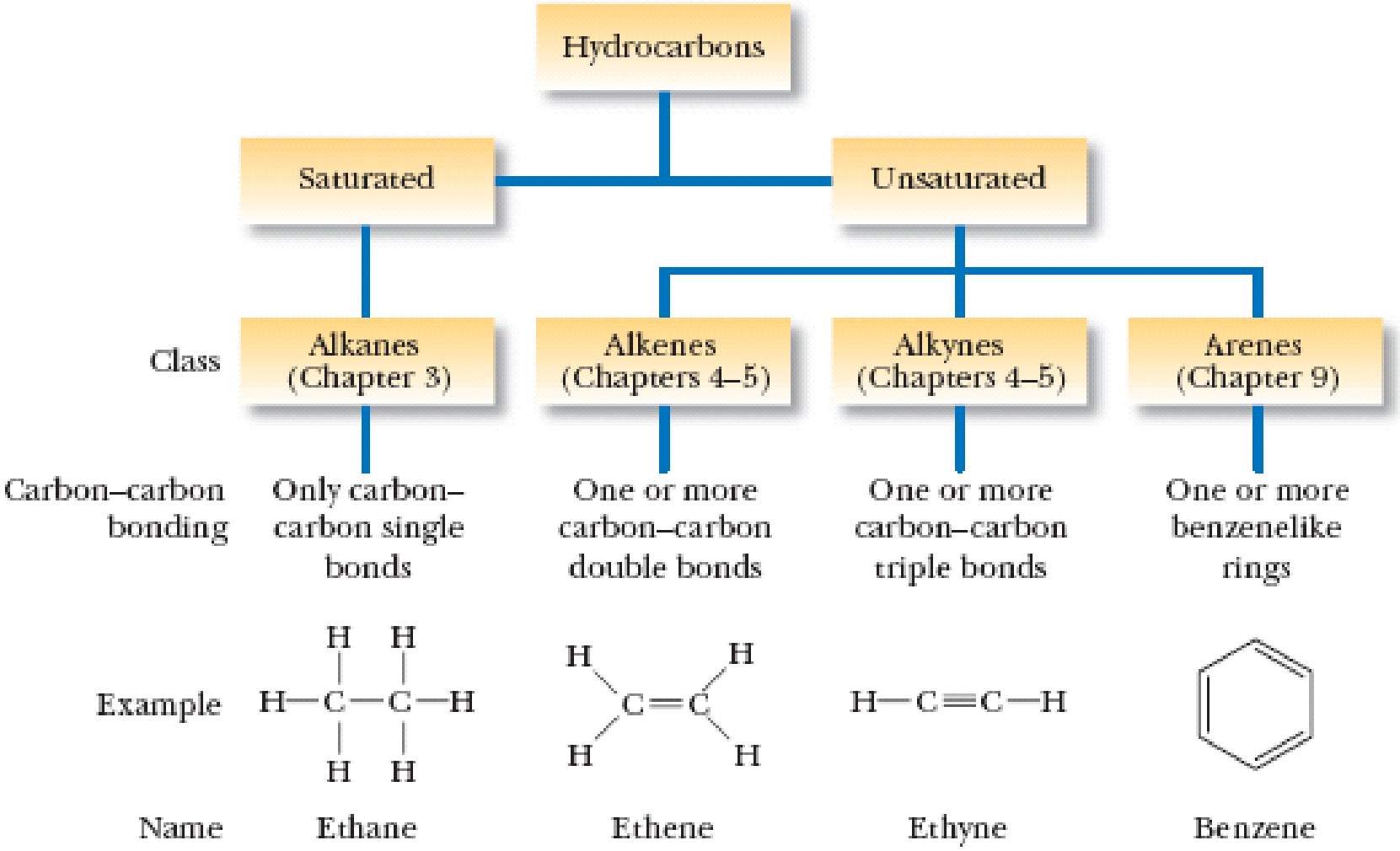
BP202TP

Chapter Three

Alkanes and Cycloalkanes

Prepared by:
Ms. Krutika Poshiya
Assistant Professor
M.Pharm

Organic Chemistry

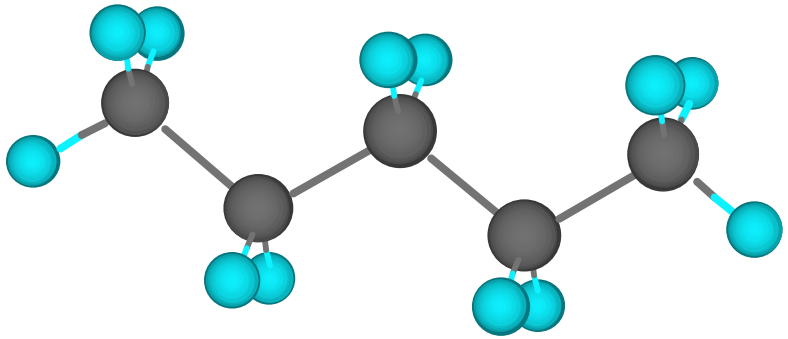


Structure

- 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 a open chain.
- Aliphatic hydrocarbon: Another name for an alkane.

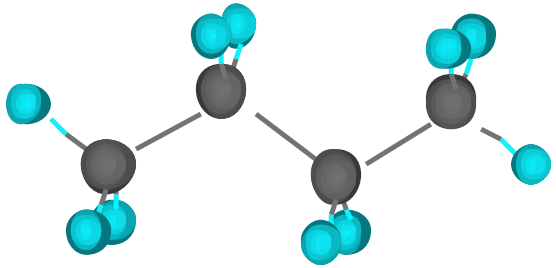
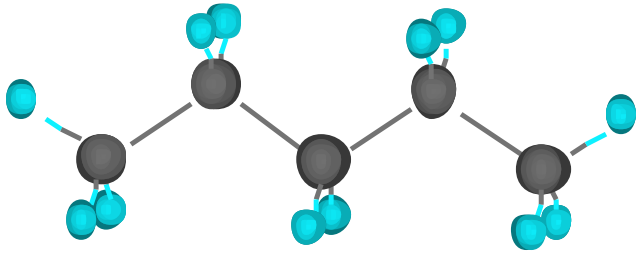
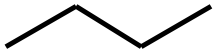
Structure

- Shape
  - Tetrahedral about carbon.
  - All bond angles are approximately 109.5°.



Representing Alkanes

- Line-angle formula
  - Each line represents a single bond.
  - Each line ending represents a CH_3 group.
  - Each vertex (angle) represents a carbon atom.

	Butane	Pentane
Ball-and-stick model		
Line-angle formula		
Structural formula	$CH_3CH_2CH_2CH_3$	$CH_3CH_2CH_2CH_2CH_3$

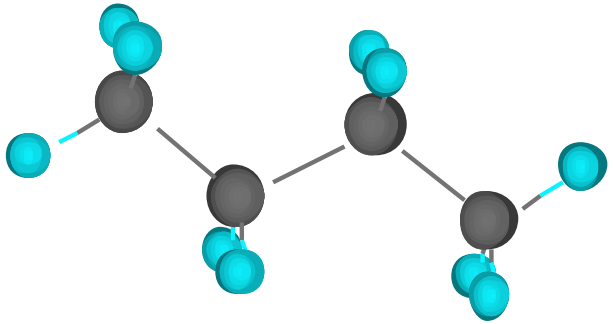
Alkanes

- Alkanes have the general formula C_nH_{2n+2}
  - Names of unbranched alkanes with 1 to 20 carbon atoms.

Name	Molecular Formula	Name	Molecular Formula
methane	CH_4	nonane	C_9H_{20}
ethane	C_2H_6	decane	$C_{10}H_{22}$
propane	C_3H_8	dodecane	$C_{12}H_{26}$
butane	C_4H_{10}	tetradecane	$C_{14}H_{30}$
pentane	C_5H_{12}	hexadecane	$C_{16}H_{34}$
hexane	C_6H_{14}	octadecane	$C_{18}H_{38}$
heptane	C_7H_{16}	eicosane	$C_{20}H_{42}$
octane	C_8H_{18}		

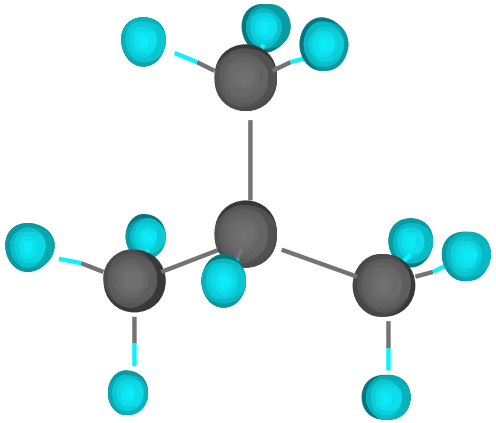
Constitutional Isomers

- **Constitutional isomers:** Compounds with the same molecular formula but a different connectivity of their atoms.
  - There are two constitutional isomers with molecular formula C_4H_{10}.



$CH_3CH_2CH_2CH_3$

Butane
(bp -0.5°C)



CH_3CHCH_3 (with CH_3 above the central C)

2-Methylpropane
(bp -11.6°C)

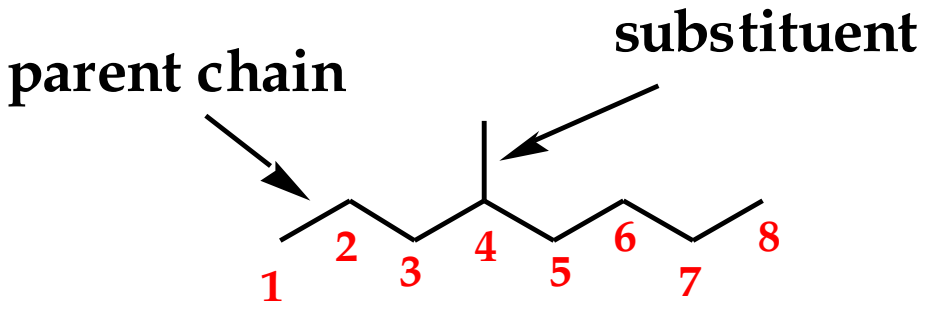
- The potential for constitutional isomerism is enormous.

Molecular Formula	Constitutional Isomers
CH_4	1
C_5H_{12}	3
$C_{10}H_{22}$	75
$C_{15}H_{32}$	4,347
$C_{25}H_{52}$	36,797,588
$C_{30}H_{62}$	4,111,846,763

World population is about 6,000,000,000

Nomenclature

- Parent name The longest carbon chain.
- Substituent: A group bonded to the parent chain.
  - Alkyl group: A substituent derived by removal of a hydrogen from an alkane; given the symbol R-.
  - CH_4 becomes CH_3- (methyl).
  - CH_3CH_3 becomes CH_3CH_2- (ethyl).



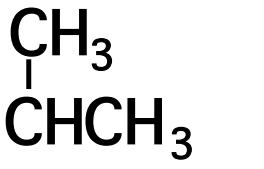
4-Methyloctane

Nomenclature

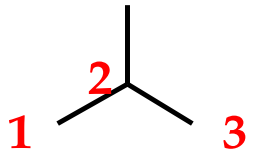
1.The name of an alkane with an unbranched chain consists of a prefix and the suffix ane.

2. For branched alkanes, the parent chain is the longest chain of carbon atoms.

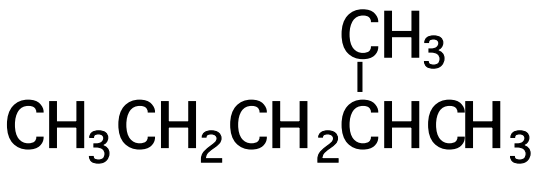
3. Each substituent is given a name and a number.



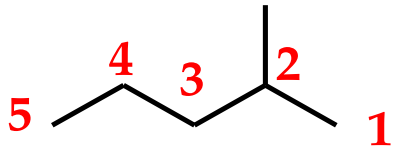
2-Methylpropane



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

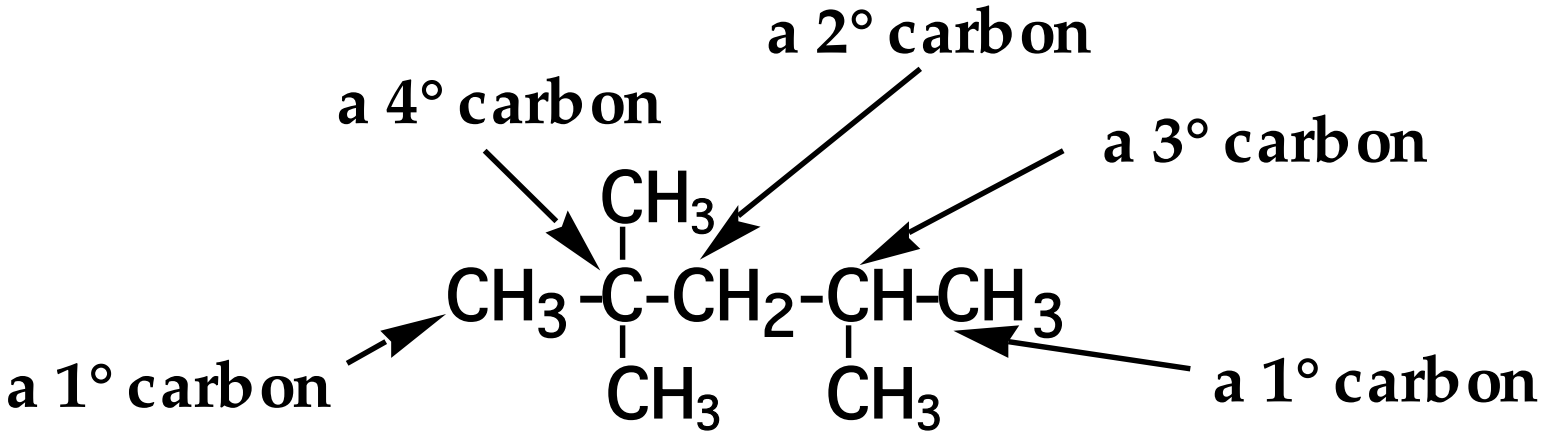


2-Methylpentane



Classification of Carbons

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



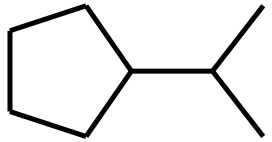
2,2,4-Trimethylpentane

Cycloalkanes

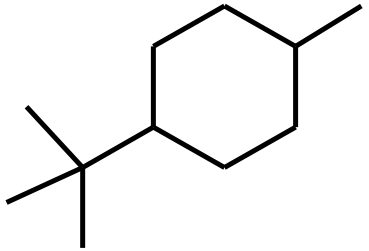
- General formula C_nH_{2n}
  - Five- and six-membered rings are the most common.
- Structure and nomenclature
  - To name, prefix the name of the corresponding open-chain alkane with cyclo-, and name each substituent on the ring.
  - If there is only one substituent, no need to give it a number.
  - If there are two substituents, number from the substituent of lower alphabetical order.
  - If there are three or more substituents, number to give them the lowest set of numbers, and then list substituents in alphabetical order.

Cycloalkanes

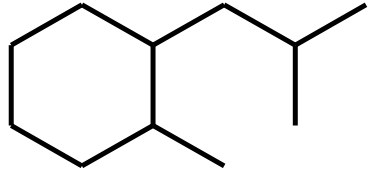
- Commonly written as line-angle formulas
  - examples:



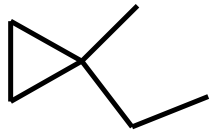
Isopropylcyclopentane



1-*tert*-Butyl-4-methyl-cyclohexane



1-Isobutyl-2-methyl-cyclohexane



1-Ethyl-1-methyl-cyclopropane

A General System

- prefix-infix-suffix
  - Prefix tells the number of carbon atoms in the parent.
  - Infix tells the nature of the carbon-carbon bonds.
  - Suffix tells the class of 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 of Compound
-e	hydrocarbon
-ol	alcohol
-al	aldehyde
-one	ketone
-oic acid	carboxylic acid

A general system

prop-en-e = propene

eth-an-ol = ethanol

but-an-one = butanone

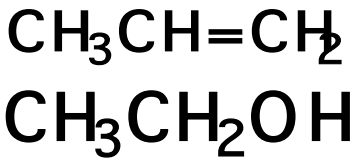
but-an-al = butanal

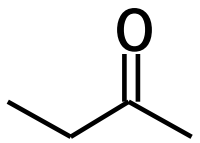
pent-an-oic acid = pentanoic acid

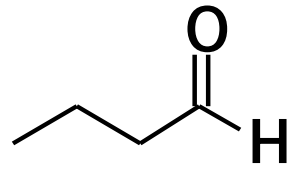
cyclohex-an-ol = cyclohexanol

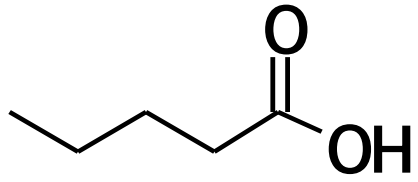
eth-yn-e = ethyne

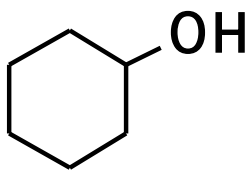
eth-an-amine = ethanamine





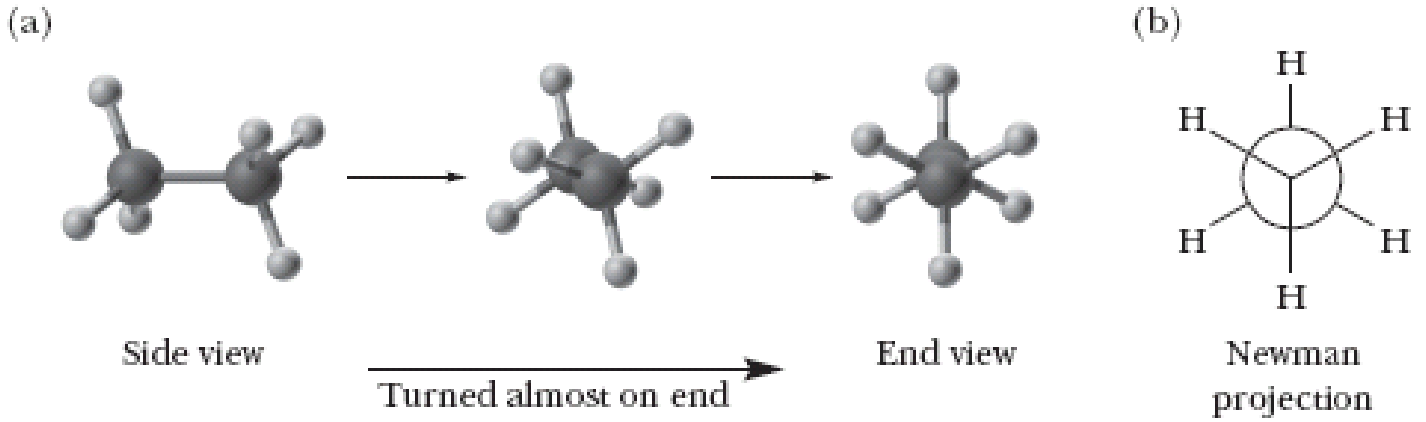






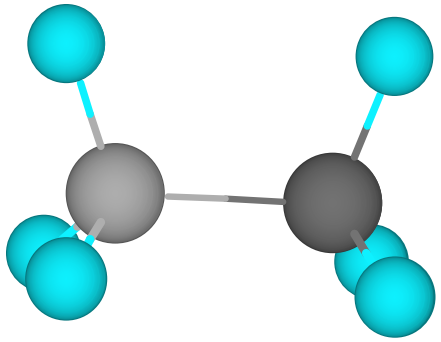
Conformation

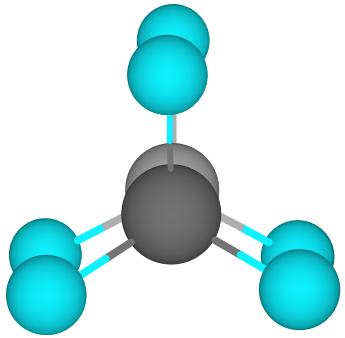
- Conformation: Any three-dimensional arrangement of atoms in a molecule that results from rotation about a single bond.
  - Staggered conformation: A conformation about a carbon-carbon single bond where the atoms on one carbon are as far apart as possible from the atoms on an adjacent carbon. On the right is a Newman projection formula.

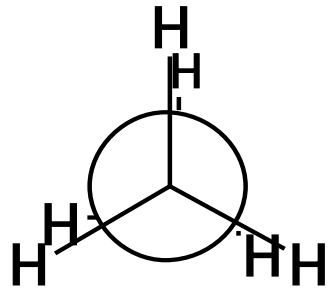


Conformation

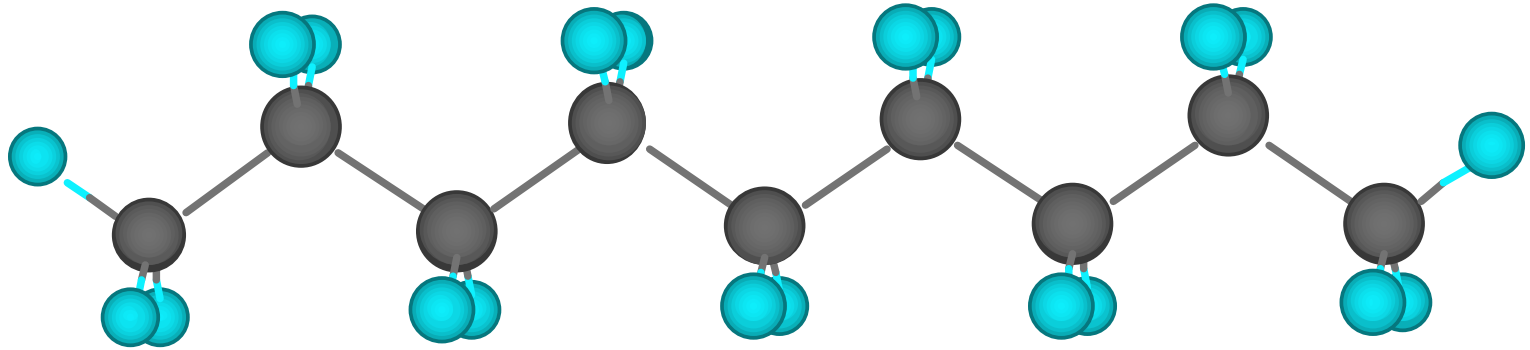
- Eclipsed conformation: A conformation about a carbon-carbon single bond in which the atoms on one carbon are as close as possible to the atoms on an adjacent carbon.







- The lowest energy conformation of an alkane is a fully staggered conformation.



Physical Properties

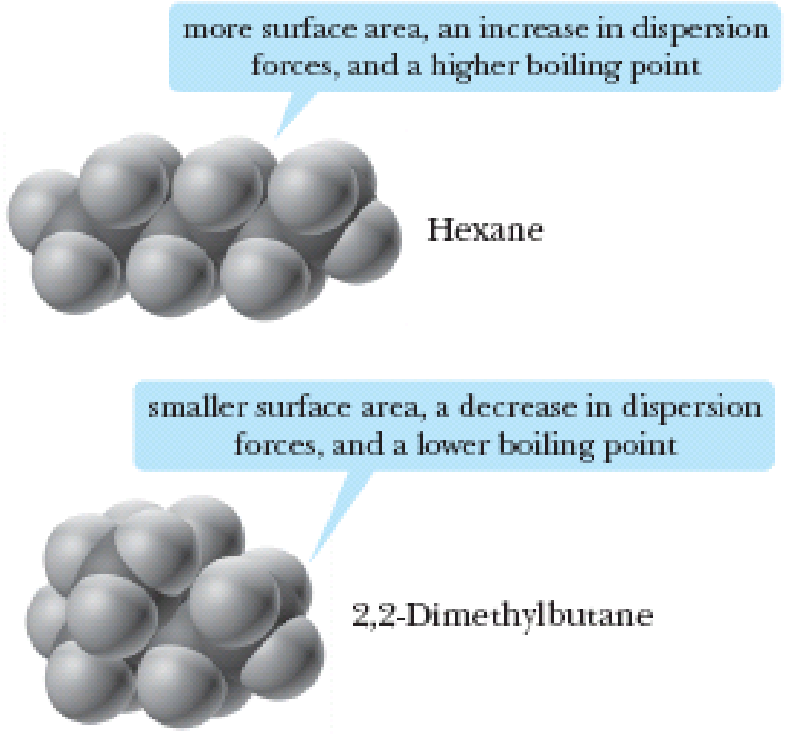
- Boiling point
  - Low-molecular-weight alkanes (1 to 4 carbons) are gases at room temperature; e.g., methane, propane, butane.
  - Higher-molecular-weight alkanes (5 to 17 carbons) are liquids at room temperature (e.g., hexane, decane, gasoline, kerosene).
  - High-molecular-weight alkanes (18 or more carbons) are white, waxy semisolids or solids at room temperature (e.g., paraffin wax).
- Density
  - Average density is about 0.7 g/mL.
  - Liquid and solid alkanes float on water.

Physical Properties

- Constitutional isomers are different compounds and have different physical properties.

TABLE 3.5 Physical Properties of the Isomeric Alkanes with the Molecular Formula C_6H_{14}

Name	Melting Point (°C)	Boiling Point (°C)	Density (g/mL)
hexane	−95	69	0.659
3-methylpentane	−6	64	0.664
2-methylpentane	−23	62	0.653
2,3-dimethylbutane	−129	58	0.662
2,2-dimethylbutane	−100	50	0.649



Reactions of Alkanes

- Oxidation is the basis for the use of alkanes as energy sources for heat and power.
  - Heat of combustion: the heat released when one mole of a substance is oxidized to carbon dioxide and water.

$$\underset{\text{Methane}}{CH_4} + 2O_2 \longrightarrow CO_2 + 2H_2O \qquad \Delta H^\circ = -886 \text{ kJ/mol } (-212 \text{ kcal/mol})$$

$$\underset{\text{Propane}}{CH_3CH_2CH_3} + 5O_2 \longrightarrow 3CO_2 + 4H_2O \qquad \Delta H^\circ = -2{,}220 \text{ kJ/mol } (-530 \text{ kcal/mol})$$