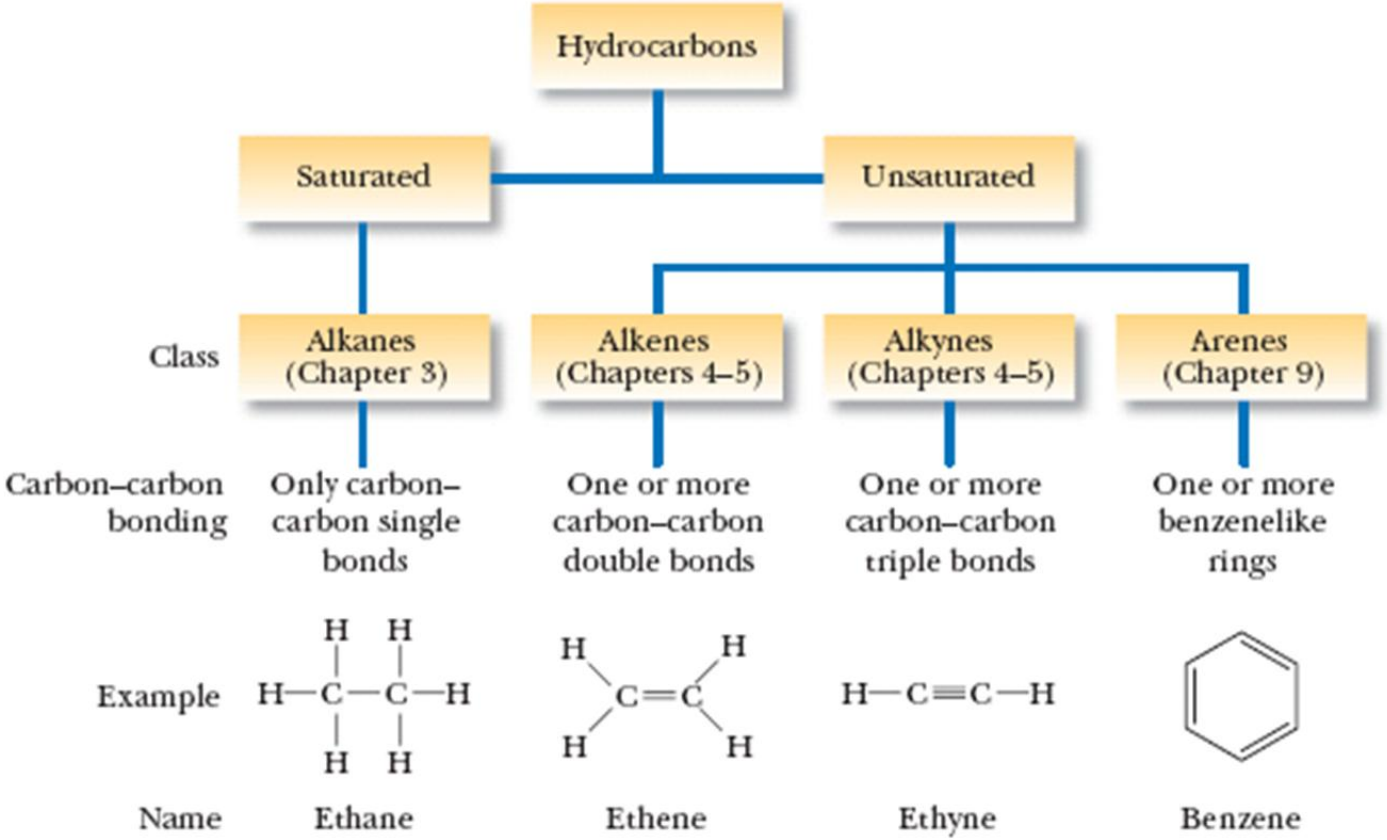
Alkanes and Cycloalkanes

Organic Chemistry

Families of Organic Compounds

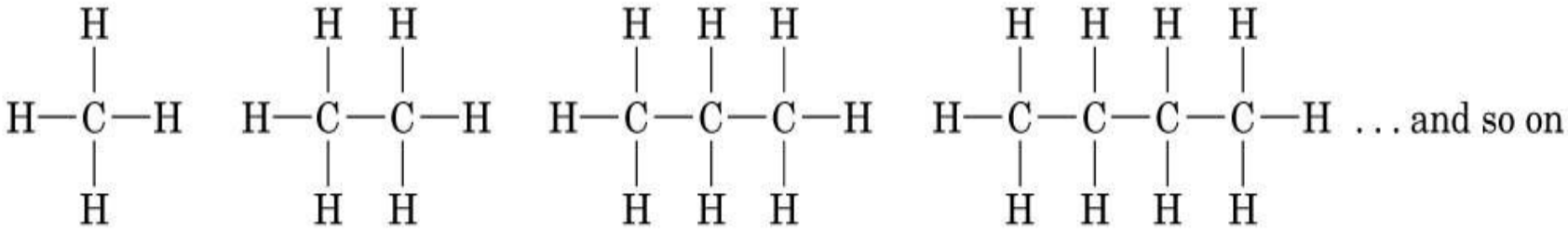
- Organic Chemistry
  - The study of carbon-containing compounds and their properties. The vast majority of organic compounds contain chains or rings of carbon atoms.
- Hydrocarbon: A compound composed only of carbon and hydrogen.
- Saturated hydrocarbon: A hydrocarbon containing only single bonds.
- Alkane: A saturated hydrocarbon whose carbons are arranged in a open chain.
- Aliphatic hydrocarbon: Another name for an alkane
- This lecture deals with ***alkanes***, compounds that contain only carbons and hydrogen's, all connected exclusively by single bonds

Organic Chemistry



2.2 Alkanes and Alkane Isomers

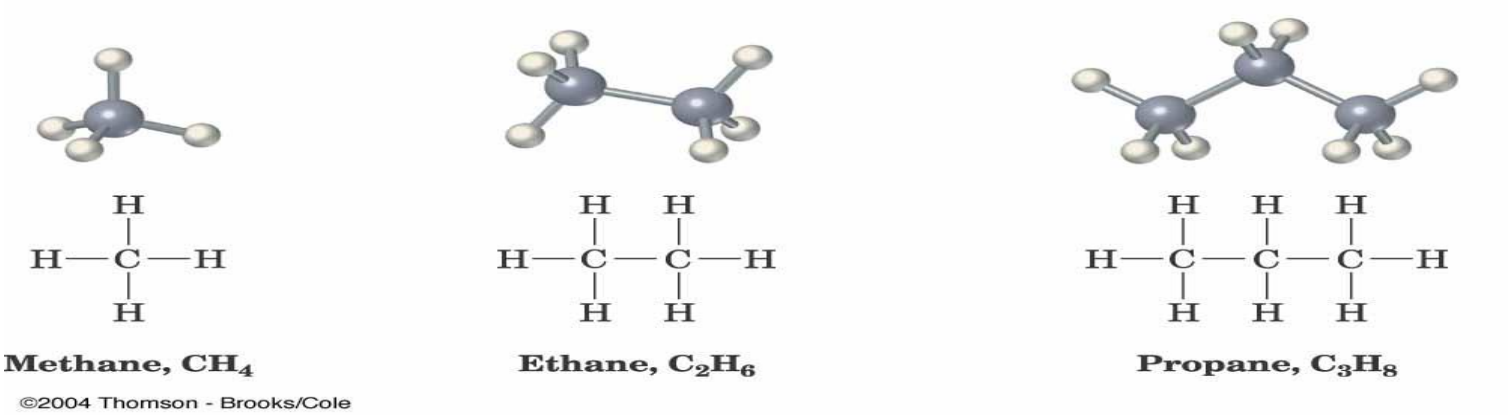
- Alkanes: Compounds with C-C single bonds and C-H bonds only (no functional groups)
- The formula for an alkane with no rings (acyclic) must be $\mathbf{C_nH_{2n+2}}$ where the number of C's is n (n is any integer)
- Alkanes are **saturated** with hydrogen (no more can be added)
- They are also called **aliphatic compounds**



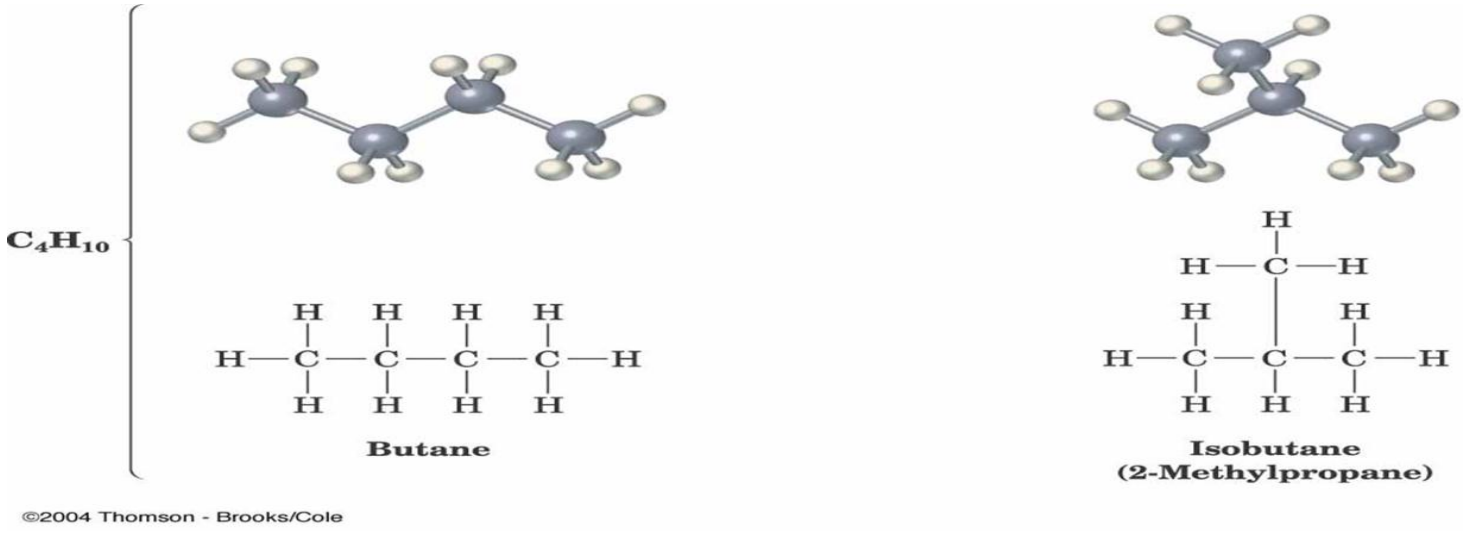
Alkane Isomers

- CH_4 = methane, C_2H_6 = ethane, C_3H_8= propane
- The molecular formula of an alkane with more than three carbons can give more than one structure
  - C_4 (butane) = butane and isobutane
  - C_5 (pentane) = pentane, 2-methylbutane (isopentane), and 2,2-dimethylpropane (neopentane)

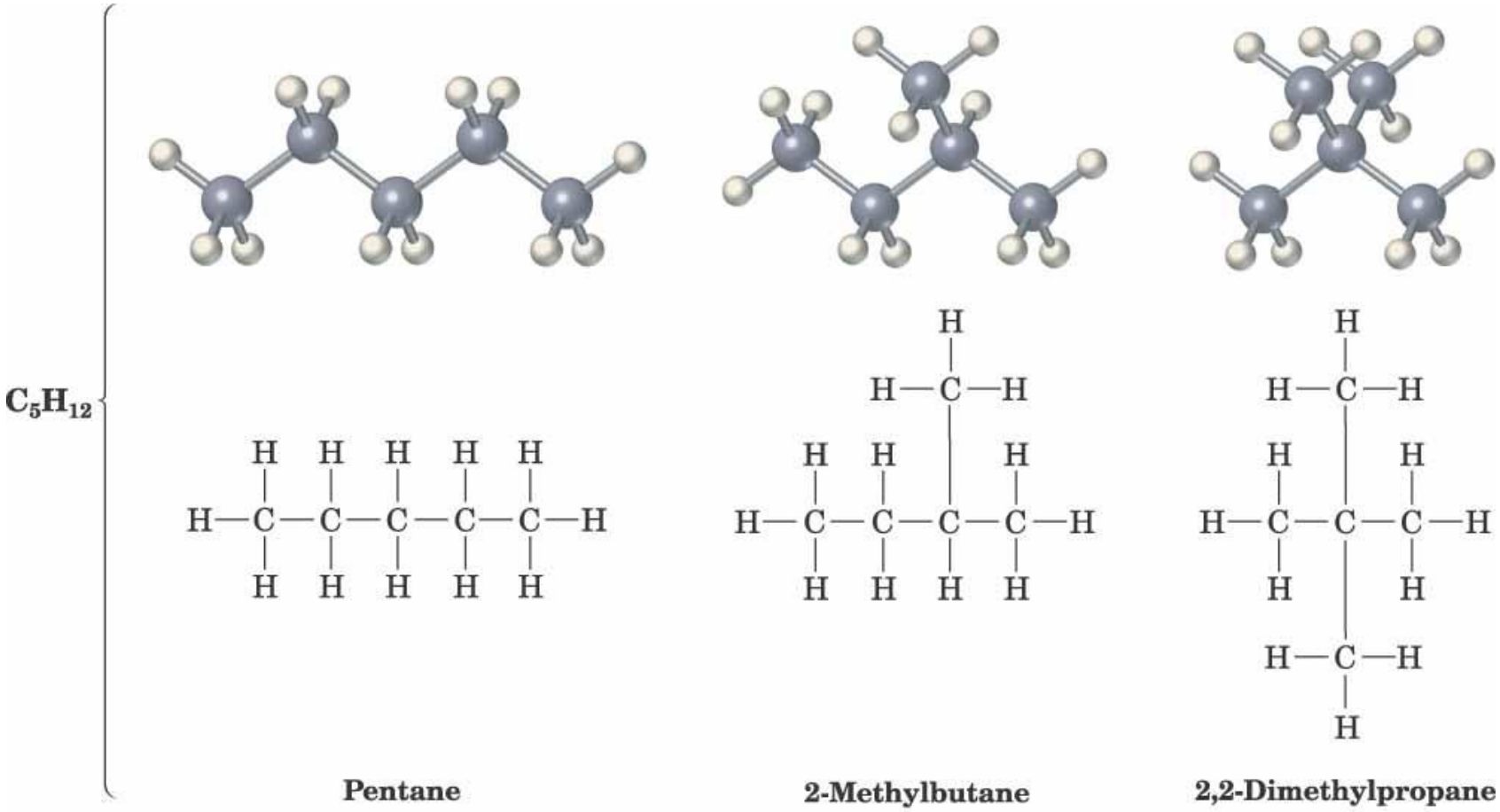
Methane, ethane, & propane



Butanes (C_4H_{10}):



Pentanes (C_5H_{12}):



Alkane Isomers

- Alkanes with C's connected to no more than 2 other C's are **straight-chain** or **normal alkanes**
- Alkanes with one or more C's connected to 3 or 4 C's are **branched-chain alkanes**
- Isomers that differ in how their atoms are arranged in chains are called constitutional (or structural) isomers
- Compounds other than alkanes can also be constitutional isomers of one another
- They must have the same molecular formula to be isomers
- We can represent an alkane in a brief form or in many types of extended form a condensed structure does not show bonds but lists atoms, such as
- CH3CH2CH3 (propane)
- CH3(CH2)2CH3 (2,2-dimethylpropane)

Names of Small Hydrocarbons

No. of Carbons	Formula Name	(C_nH_{2n+2})
1	Methane	CH_4
2	Ethane	C_2H_6
3	Propane	C_3H_8
4	Butane	C_4H_{10}
5	Pentane	C_5H_{12}
6	Hexane	C_6H_{14}
7	Heptane	C_7H_{16}
8	Octane	C_8H_{18}
9	Nonane	C_9H_{20}
10	Decane	$C_{10}H_{22}$

2.3 Alkyl Groups

- **Alkyl group** – remove one H from an alkane (a part of a structure)
- General abbreviation "R" (for Radical, an incomplete species or the "rest" of the molecule)
- Name: replace -*ane* ending of alkane with -*yl* ending
  - $-CH_3$ is "methyl" (from methane)
  - $-CH_2CH_3$ is "ethyl" from ethane

2.3 Alkyl Groups

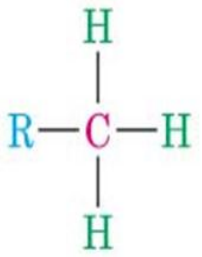
TABLE 3.4 Some Straight-Chain Alkyl Groups

Alkane	Name	Alkyl group	Name (abbreviation)
CH_4	Methane	$—CH_3$	Methyl (Me)
CH_3CH_3	Ethane	$—CH_2CH_3$	Ethyl (Et)
$CH_3CH_2CH_3$	Propane	$—CH_2CH_2CH_3$	Propyl (Pr)
$CH_3CH_2CH_2CH_3$	Butane	$—CH_2CH_2CH_2CH_3$	Butyl (Bu)
$CH_3CH_2CH_2CH_2CH_3$	Pentane	$—CH_2CH_2CH_2CH_2CH_3$	Pentyl, or amyl

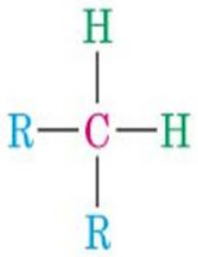
Types of Alkyl groups

- a carbon at the end of a chain (primary alkyl group)
- a carbon in the middle of a chain (secondary alkyl group)
- a carbon with three carbons attached to it (tertiary alkyl group)

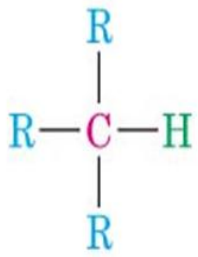
Types of Carbon Atoms



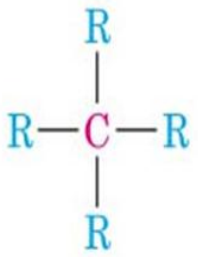
Primary **carbon (1°) is bonded to one other carbon**



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



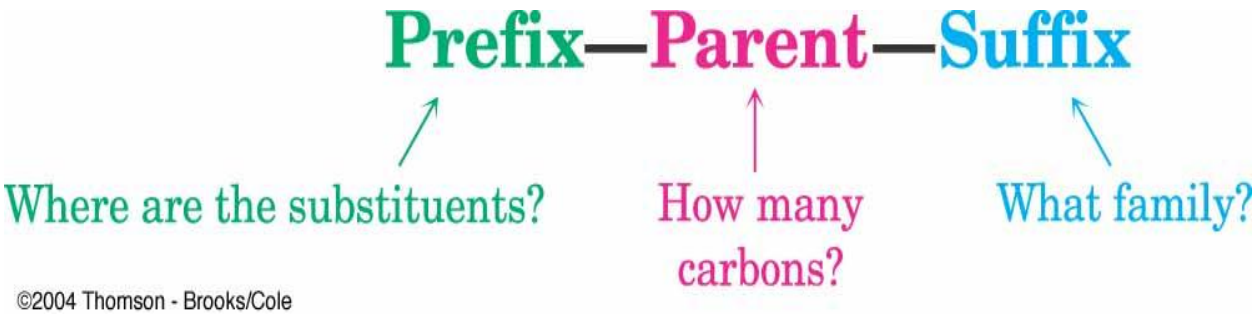
Tertiary **carbon (3°) is bonded to three other carbons**



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

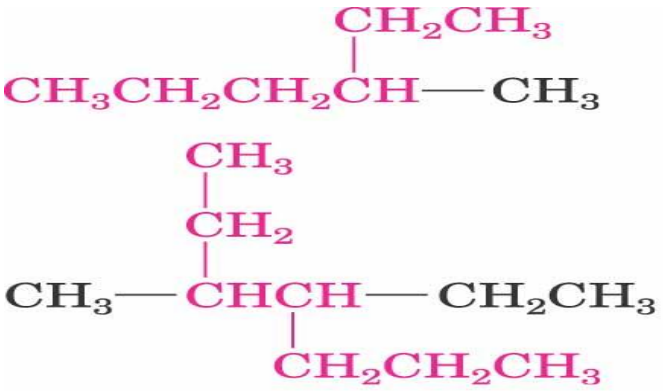
2.4 Naming Alkanes: IUPAC

- Compounds are given systematic names by a process that uses:



  - Follows specific rules
    - Named as longest continuous chain of C's
    - Carbons in that chain are numbered in sequence
    - Substituents are numbered at their point of attachment
    - Complex substituents are named similarly

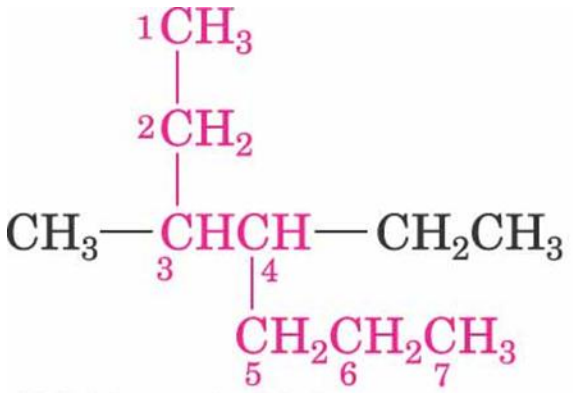
1. Find the Parent: longest continuous carbon chain



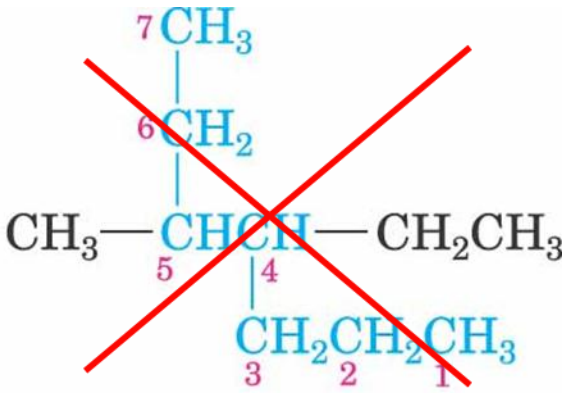
Named as a substituted hexane

Named as a substituted heptane

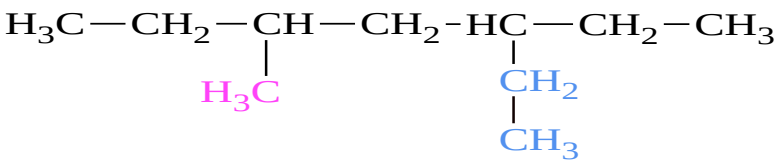
2. Number the atoms in the chain with the end of the chain nearer the first substituent



NOT

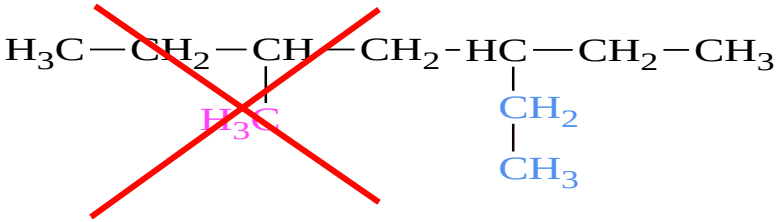


3. **Identify & number the substituents. When two substituents are present at an equal distance from either end of the longest chain, we number the ring beginning with the substituent first in the alphabet. In deciding on alphabetical oreder disregard multiplying prefixes such as "di" and "tri" etc. and the prefixes like *sec*- or *tert*.**



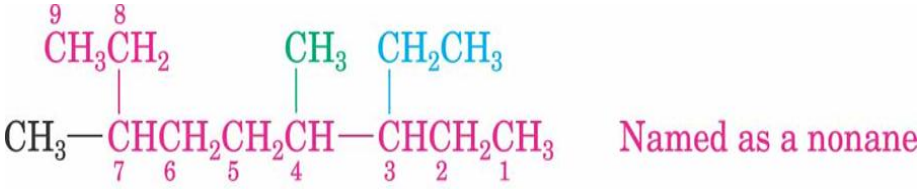
3-Ethyl-5-methylheptane

NOT

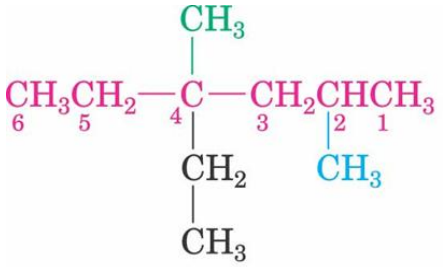


3-Methyl-5-ethylheptane

4. When three or more substituents are present, we begin at the substituent that leads to the lowest set of locants.

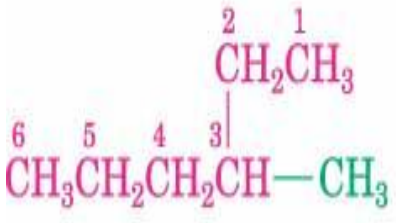


Substituents: On C3, CH_2CH_3 (3-ethyl)
On C4, CH_3 (4-methyl)
On C7, CH_3 (7-methyl)

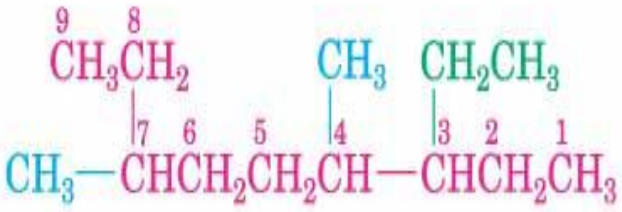


Substituents: On C2, CH_3 (2-methyl)
On C4, CH_3 (4-methyl)
On C4, CH_2CH_3 (4-ethyl)

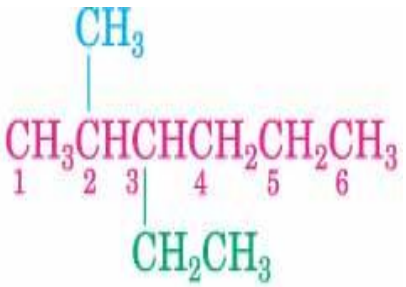
4. Write the name



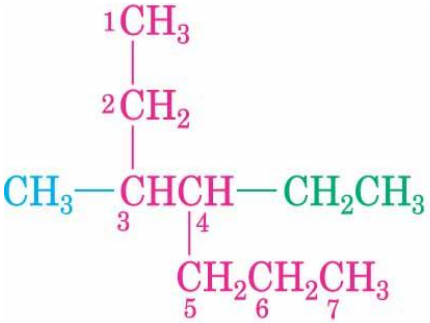
3-Methylhexane



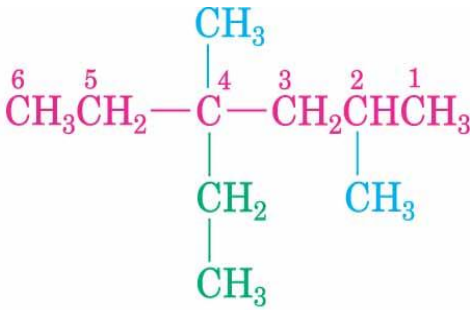
3-Ethyl-4,7-dimethylnonane



3-Ethyl-2-methylhexane

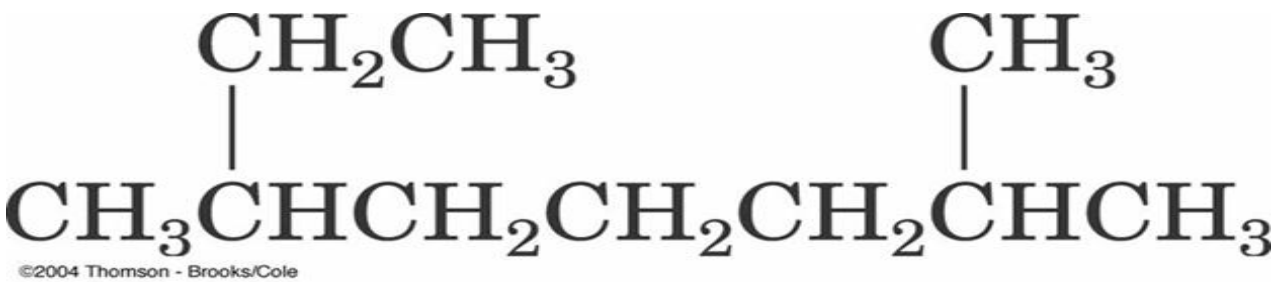


4-Ethyl-3-methylheptane

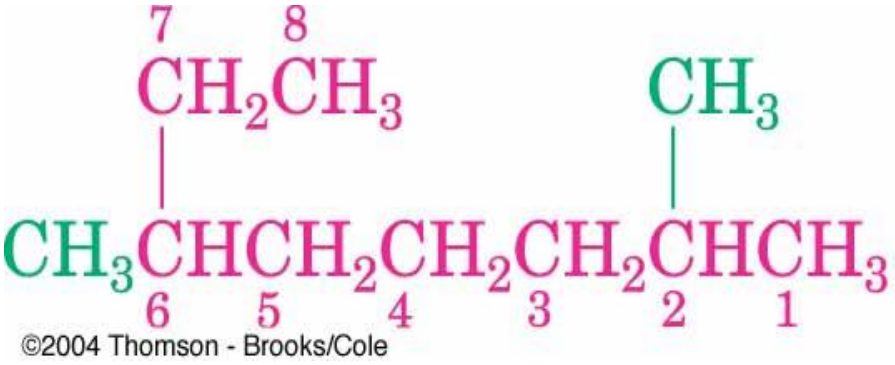


4-Ethyl-2,4-dimethylhexane

Practice problem : IUPAC name?



Solution:



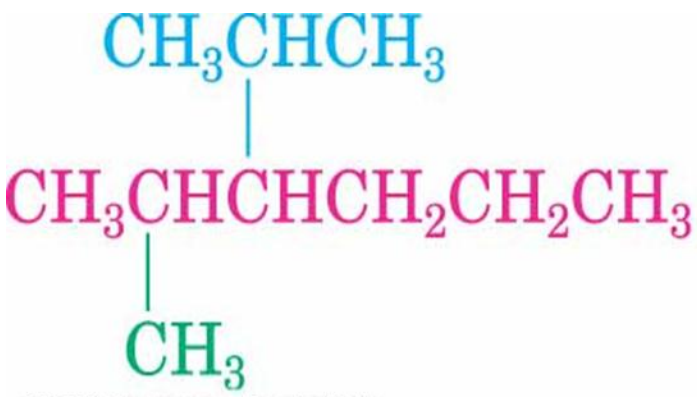
2,6-Dimethyloctane

Practice : structure?

3-isopropyl-2-methylhexane

- C-C-C-C-C-C
- Two substituents: isopropyl & methyl
- Add hydrogens to complete the structure

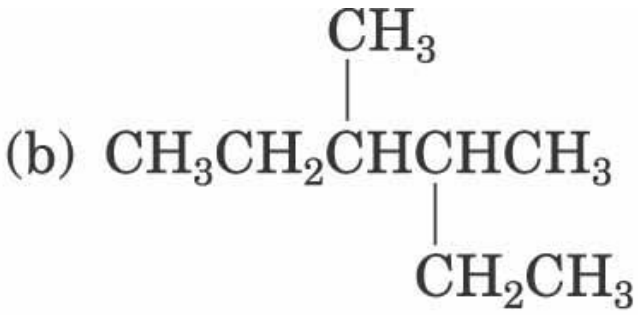
Solution:



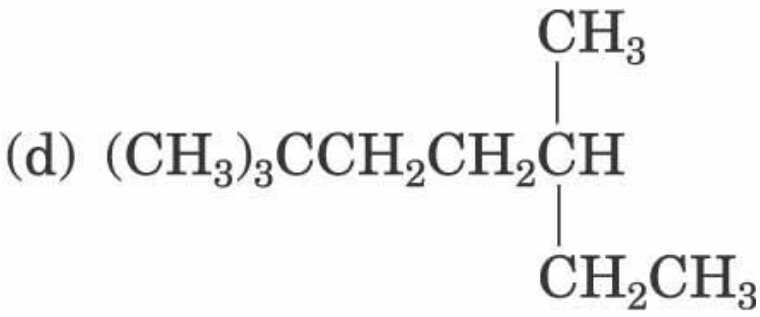
3-Isopropyl-2-methylhexane

Problem : IUPAC names?

(a) The three isomers of C_5H_{12}

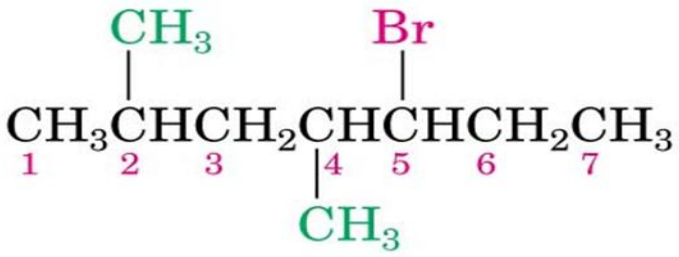
(b) 

(c) 

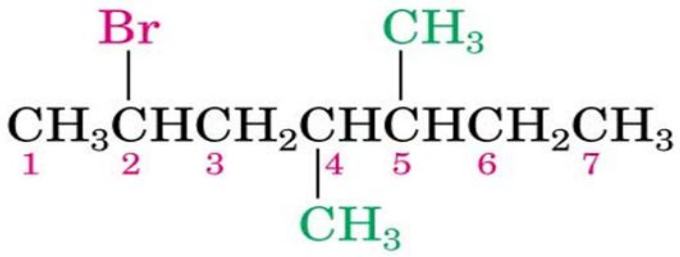
(d) 

2.5 Naming Alkyl Halides

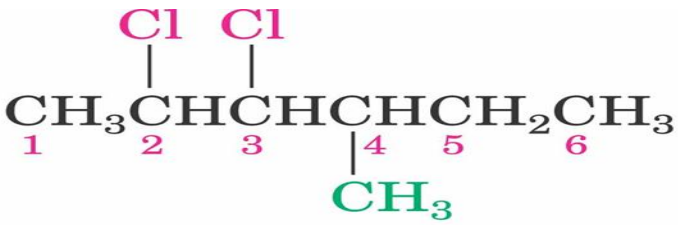
- Name is based on longest carbon chain
  - (Contains double or triple bond if present)
  - Number from end nearest any substituent (alkyl or halogen)
  - Halogens have same priority as alkyl groups



5-Bromo-2,4-dimethylheptane



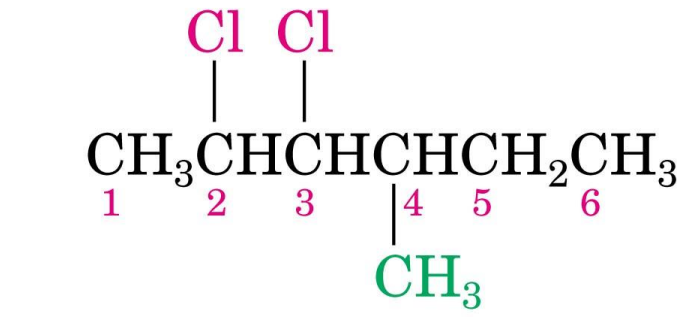
2-Bromo-4,5-dimethylheptane



2,3-Dichloro-4-methylhexane

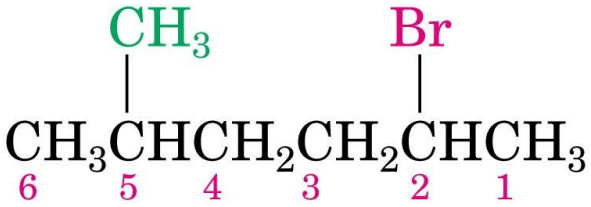
Naming with Multiple Halides

- If more than one of the same kind of halogen is present, use prefix *di, tri, tetra*



2,3-Dichloro-4-methylhexane

- If there are several different substituents (halogens or alkyls), number them and list them in alphabetical order



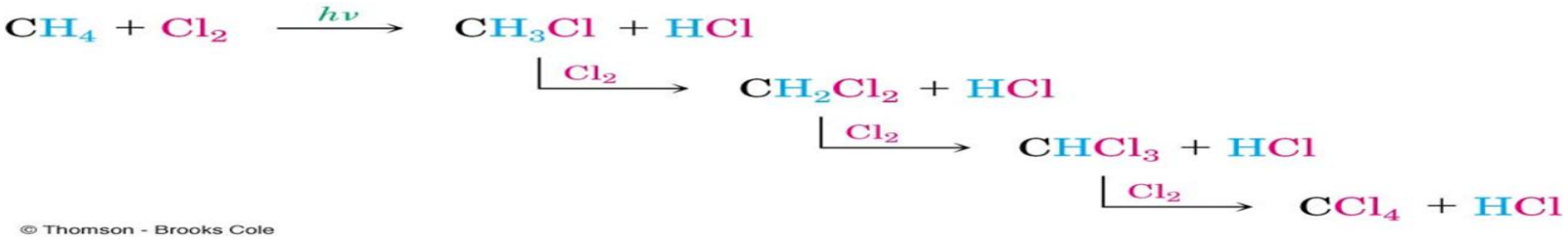
2-Bromo-5-methylhexane
(*NOT* 5-bromo-2-methylhexane)

2.6 Properties of Alkanes

- Called **paraffin's** (low affinity compounds) because they are relatively unreactive
- They will burn in a flame, producing carbon dioxide, water, and heat

$$CH_4 + 2\,O_2 \rightarrow CO_2 + 2\,H_2O + \text{heat}$$

- They react with Cl2 in the presence of light to replace H's with Cl's (not easily controlled)



Physical Properties

Boiling points and melting points increase as size of alkane increases
Forces between molecules (temporary dipoles, dispersion) are weak

Physical Properties

- Alkanes are nonpolar compounds and have only weak interactions between their molecules.
- Dispersion forces: Weak intermolecular forces of attraction resulting from interaction of temporary induced dipoles.
- 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

Reactions of Alkanes

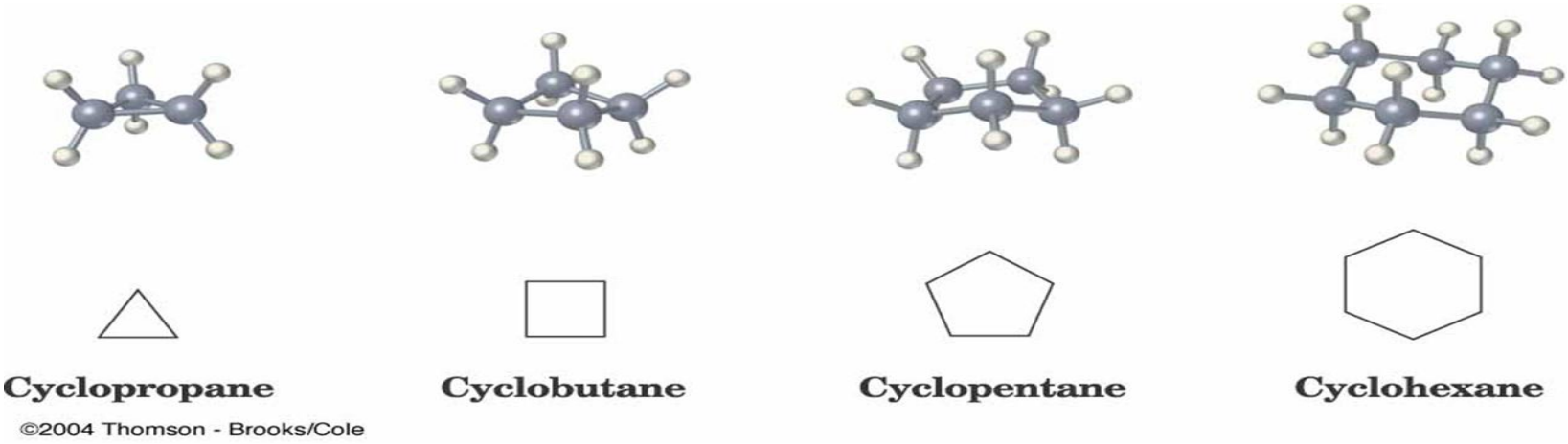
- Oxidation is the basis for the use of alkanes as energy sources for heat and power.
  - Heat of combustion: the heat released when one mole of a substance is oxidized to carbon dioxide and water.

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

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

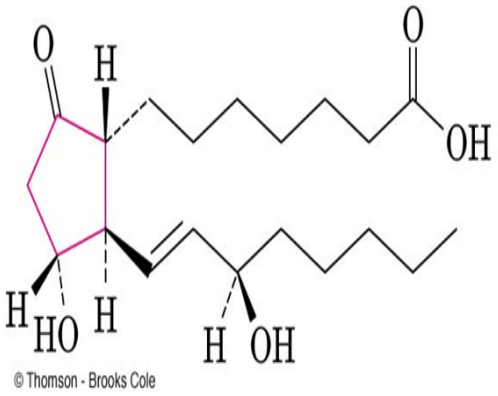
2.7 Cycloalkanes

- **Cycloalkanes** are alkanes that have carbon atoms that form a ring (called alicyclic compounds)
- Simple cycloalkanes are 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)

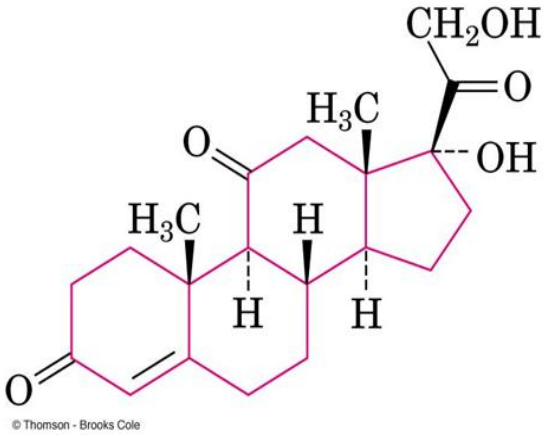


Complex Cycloalkanes

- Naturally occurring materials contain cycloalkane structures
- Examples:
  - chrysanthemic acid (cyclopropane),
  - prostaglandins (cyclopentane),
  - steroids (cyclohexanes and cyclopentane)



Prostaglandin E_1 (PGE_1)

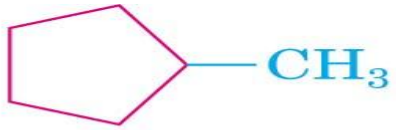


Cortisone

2.8Naming Cycloalkanes

- Count the number of carbon atoms in the ring and the number in the largest substituent chain. *If the number of carbon atoms in the ring is equal to or greater than the number in the substituent, the compound is named as an alkyl-substituted cycloalkane.*
- For an alkyl- or halo-substituted cycloalkane, start at a point of attachment as C1 and number the substituents on the ring so that the *second* substituent has as low a number as possible. When two substituents are present, we number the ring *beginning with the substituent first in the alphabet*.
- When three or more substituents are present, we begin at the substituent that leads to the lowest set of locants
- Number the substituents and write the name

1. Find the parent:



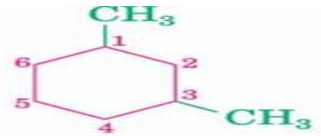
Methylcyclopentane

BUT

1-Cyclopropylbutane

or butylcyclopropane

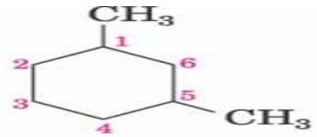
2. Number the substituents & write the name:



1,3-Dimethylcyclohexane

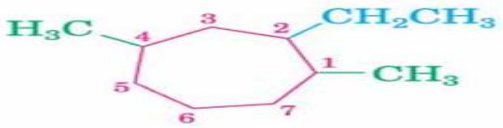
Lower

NOT



1,5-Dimethylcyclohexane

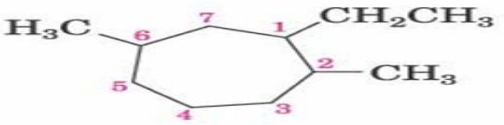
Higher



2-Ethyl-1,4-dimethylcycloheptane

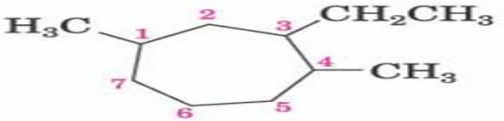
Lower Lower

NOT



1-Ethyl-2,6-dimethylcycloheptane

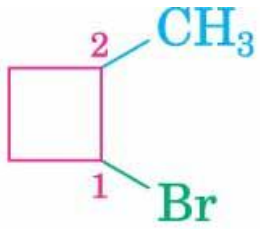
Higher



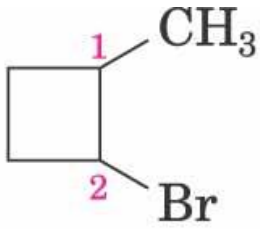
3-Ethyl-1,4-dimethylcycloheptane

Higher

Examples:

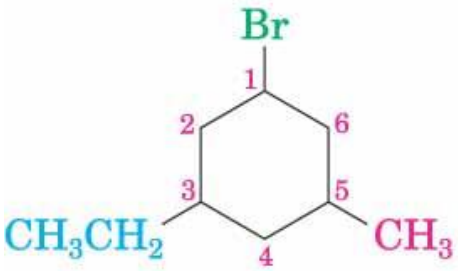


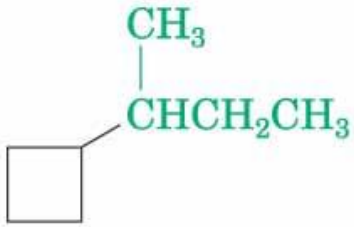
NOT

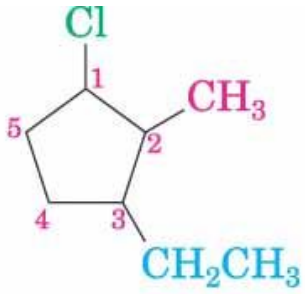


1-Bromo-2-methylcyclobutane

2-Bromo-1-methylcyclobutane





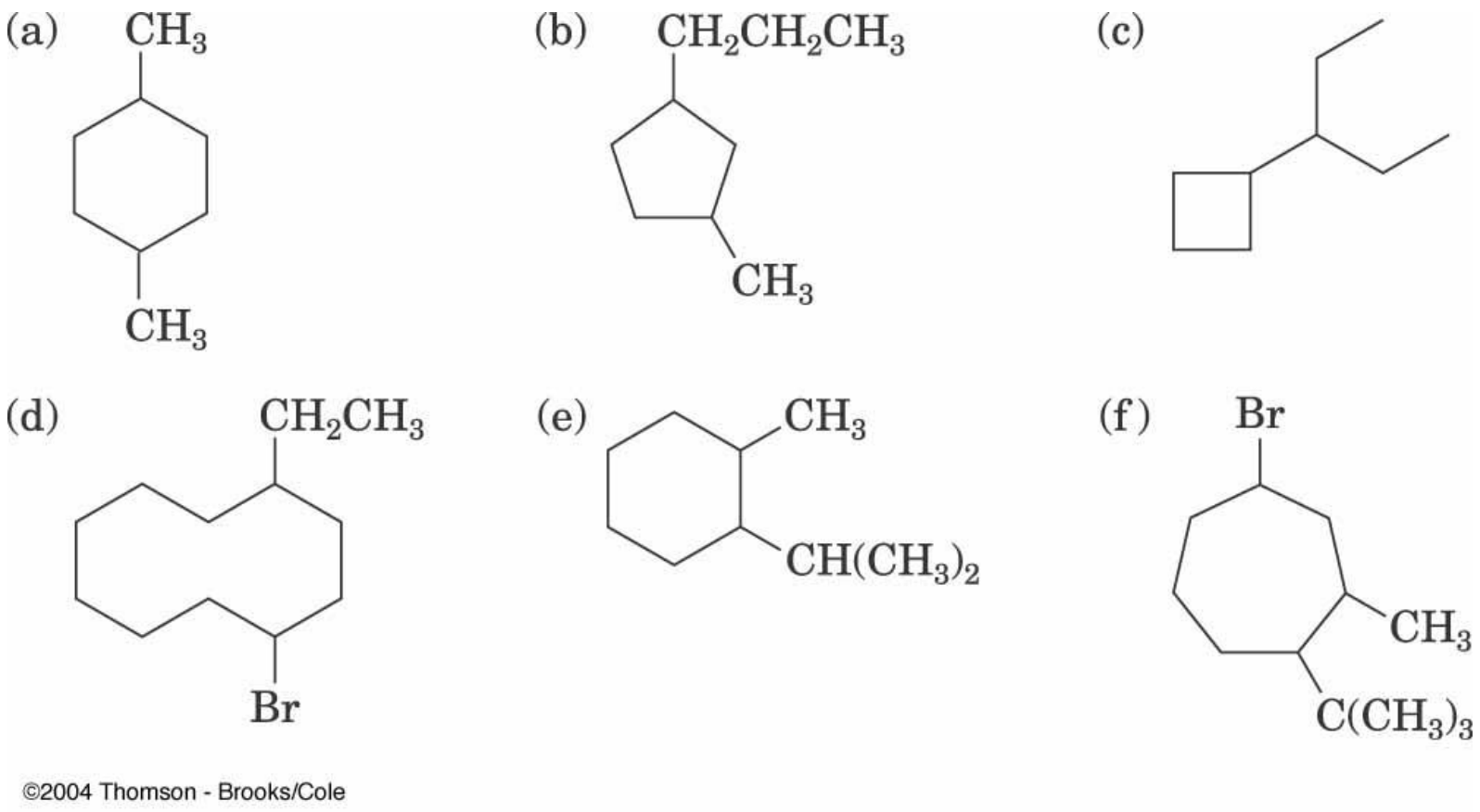


1-Bromo-3-ethyl-5-methyl-cyclohexane

(1-Methylpropyl)cyclobutane (or *sec*-Butylcyclobutane)

1-Chloro-3-ethyl-2-methyl-cyclopentane

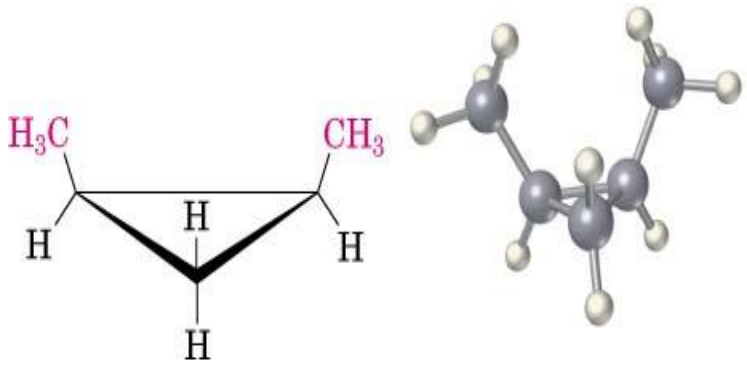
Problem : IUPAC names?



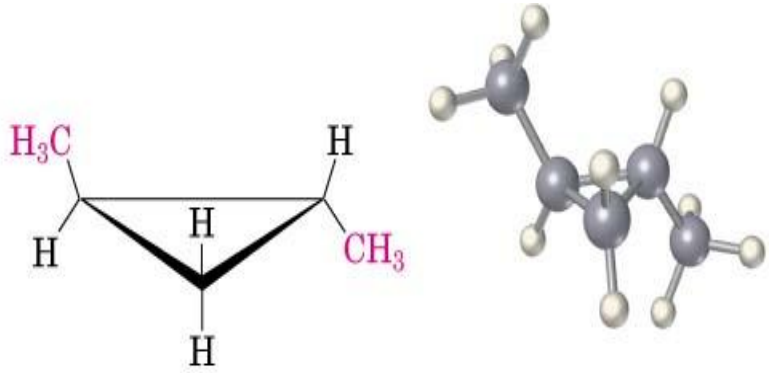
2.9 Cis-Trans Isomerism in Cycloalkanes

- Rotation about C-C bonds in cycloalkanes is limited by the ring structure
- Rings have two “faces” and substituents are labeled as to their relative facial positions
- There are two different 1,2-dimethyl-cyclopropane isomers, one with the two methyls on the same side (cis) of the ring and one with the methyls on opposite sides (trans)

2.8 Cis-Trans Isomerism in Cycloalkanes



***cis*-1,2-Dimethylcyclopropane**



***trans*-1,2-Dimethylcyclopropane**

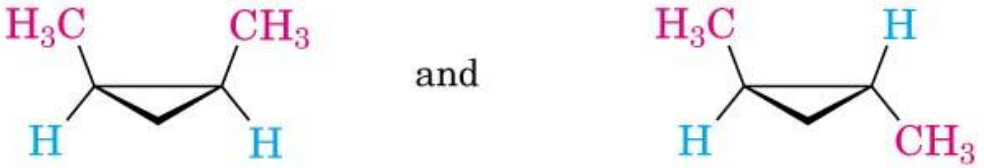
Stereoisomers

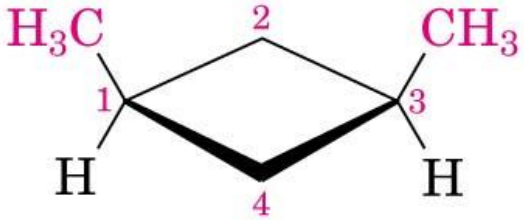
- Compounds with atoms connected in the same order but which differ in three-dimensional orientation, are **stereoisomers**
- The terms “cis” and “trans” should be used to specify stereoisomeric ring structures
- Recall that **constitutional isomers** have atoms connected in different order

Stereoisomers

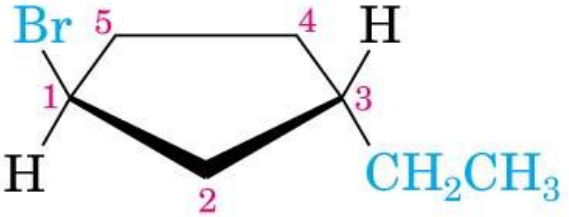
Constitutional isomers (different connections between atoms)

Stereoisomers (same connections but different three-dimensional geometry)





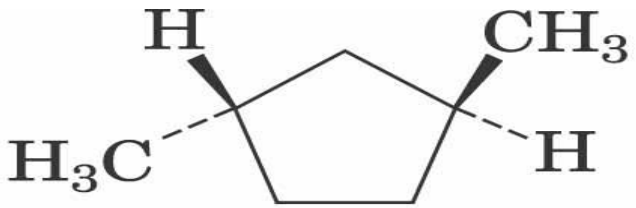
***cis*-1,3-Dimethylcyclobutane**



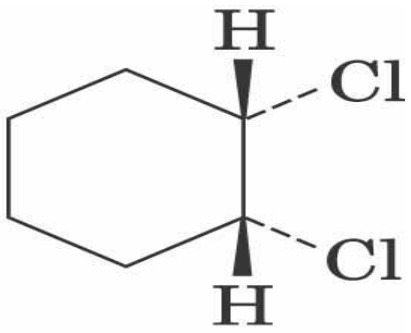
***trans*-1-Bromo-3-ethylcyclopentane**

Practice : Name?

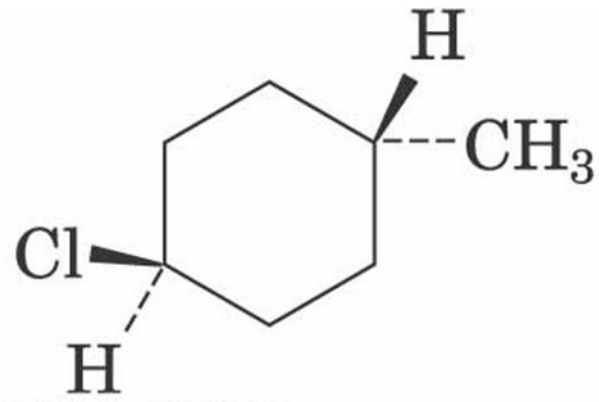
(a)



(b)



(a)



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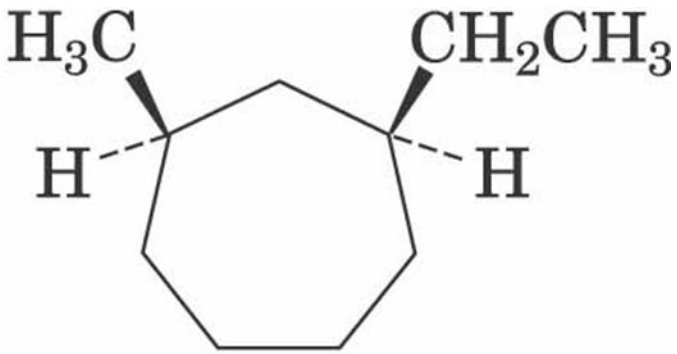

THE END