AN INTRODUCTION TO ORGANIC CHEMISTRY

By Syeda Parveen

WHAT IS ORGANIC CHEMISTRY?

- The study of carbon-containing compounds.
- General properties are different from inorganic compounds (e.g., ionic salts, etc.)

ORGANIC COMPOUNDS

- More than 9 million organic compounds are known as compared to only 500,000 known inorganic compounds.
- General properties are different from inorganic compounds (ionic salts etc.).

Organic compounds

- Covalent bonding.
- Low melting points.
- Mainly insoluble in water.
- Mainly soluble inorganic solvents (e.g., gasoline).
- Almost all burn.
- Slower reactions.

Inorganic compounds

- Ionic bonding.
- High melting points.
- Mainly soluble in water.
- Mainly insoluble in organic solvents.
- Very few burn.
- Very fast reactions.

COVALENT BONDING

- A covalent bond involves sharing of a pair of electrons between two atoms.
- Each atom contributes one electron for sharing.
- The shared electrons are localized between the two atomic nuclei.

COVALENT BONDING

Example

H2 can be represented as

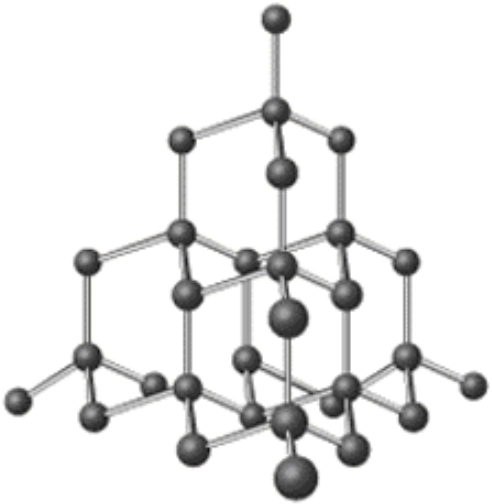
H—H

WHY CARBON?

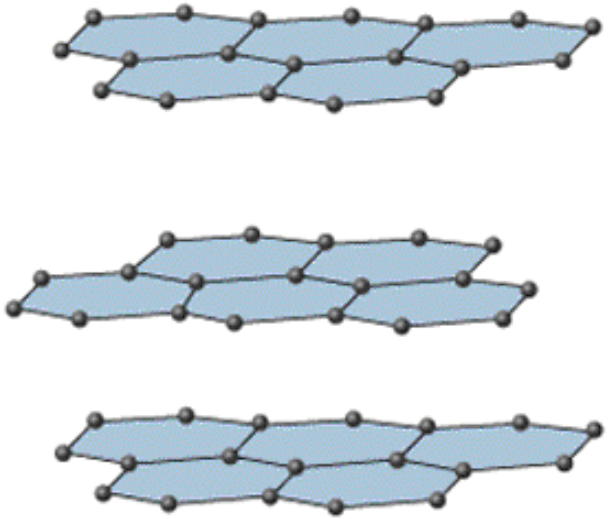
- A carbon atom forms four bonds.
- Carbon atoms form stable bonds with other carbon atoms (i.e., the C—C covalent bond is strong).
- Can form chains and even networks.
- Examples: Graphite and diamond.

WHY CARBON?

- A carbon atom forms four bonds



- Diamond



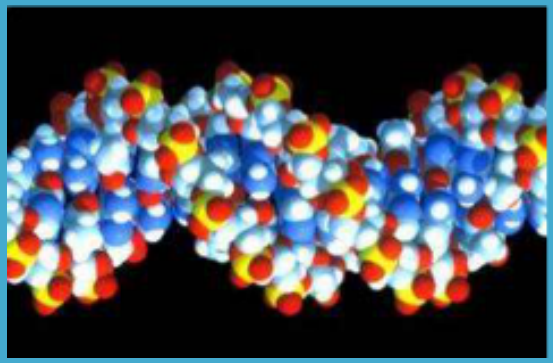
- Graphite

WHY CARBON?

- Carbon atoms also form stable bonds with other atoms (i.e., C—H, C—O, C—N, C—Cl etc. bonds are strong).
- Many combinations and arrangements are possible.

EXAMPLES OF ORGANIC COMPOUNDS

ORGANIC COMPOUNDS



DNA

Medicines

Essential Oils

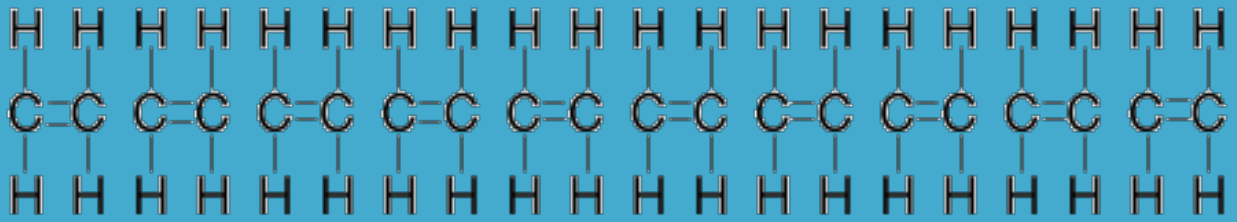
Pigments

Materials

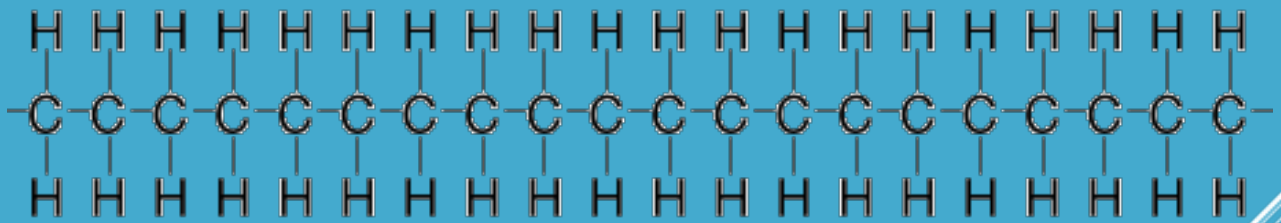
HYDROCARBONS (CnHm)

- Extracted from crude oil
- Separated according to size for various purposes
- Source of energy, plastics, solvents, raw materials, etc.

ethene molecules

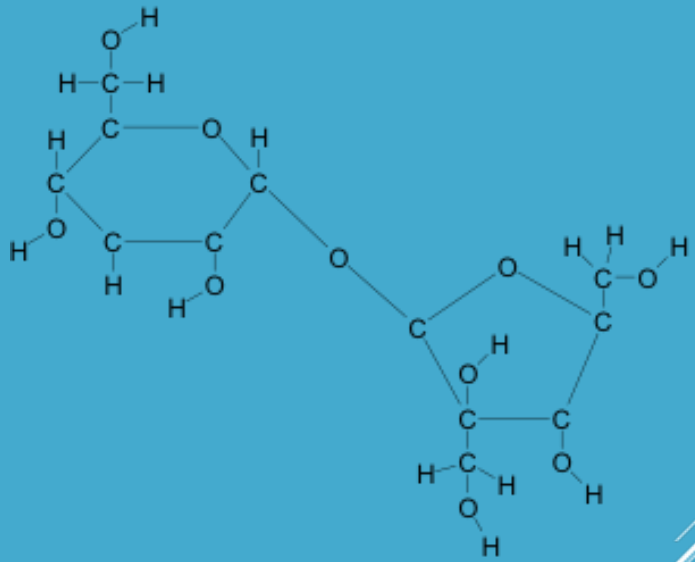


2000 atmospheres
200°C



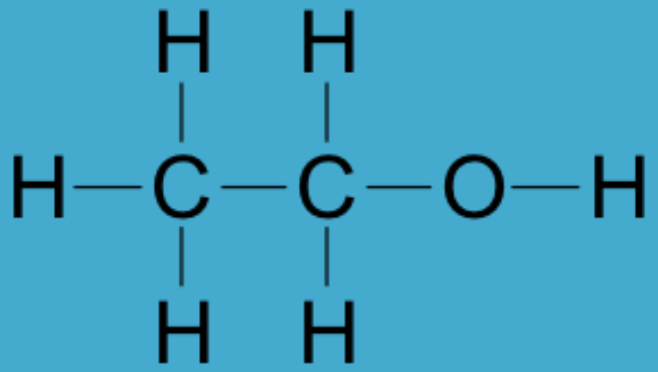
part of a polyethene molecule

SUCROSE

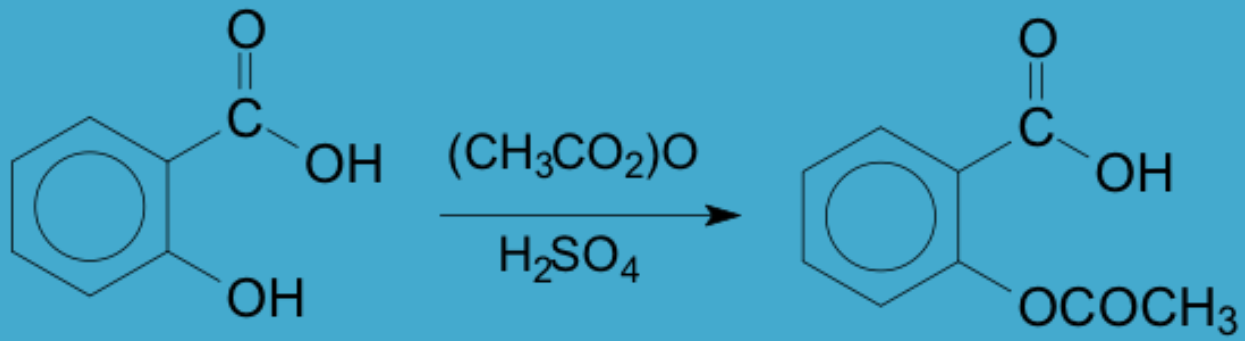


C12H22
O11

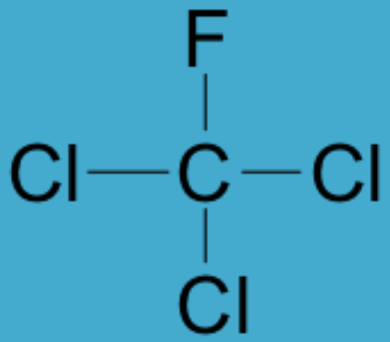
ETHANOL (C2H5OH)



ASPIRIN (ACETYLSALICYLIC ACID)



CHLOROFLUOROCARBONS(CFCS)



$CFCl_3$

WHAT ARE ORGANIC MOLECULES?

- Main structure: carbon backbone.
- Each carbon must have 4 covalent bonds (i.e., share an electron with a neighboring atom).
- Modular system, building blocks attached to each other by covalent bonds.
- Functional groups with specific properties.

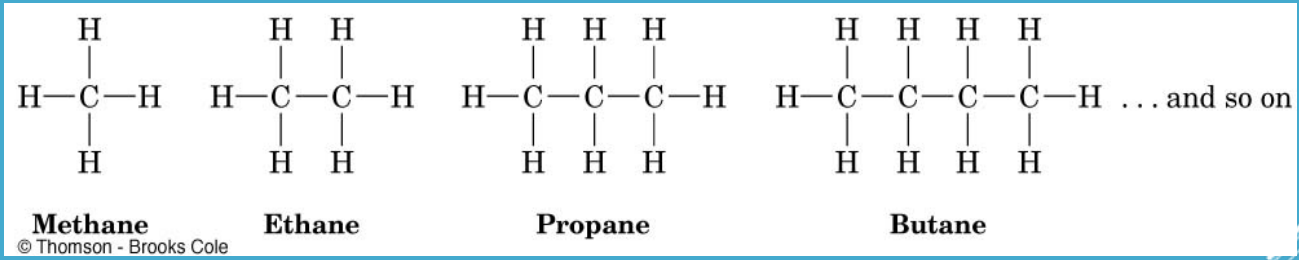
FUNCTIONAL GROUPS

A functional group is an atom or group of atoms that have a characteristic chemical behavior.

- Alcohol- R–OH
- Haloalkanes- R–X (X=F,Cl,Br,I)
- Amine- R–NH2
- Carboxylic acid- R–COOH
- Amide- R–CONH2
- Aldehyde- R-CHO
- Ketone- R-CO-R
- Ester- RCOO-R
- Ether- R-O-R
- Nitrile- R-CN
- Thiol- R-SH
- Sulphides- R-S-R
- Acid Chloride- RCOCl

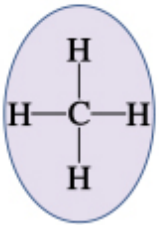
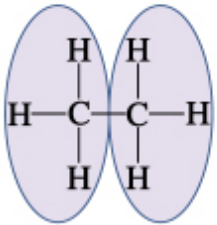
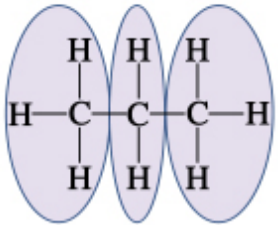
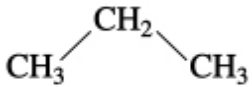
ALKANES

- Alkanes are saturated hydrocarbons with C-C single bonds and C-H bond only.
- General formula of alkanes is CnH2n+2
- They are also called as aliphatic compounds.



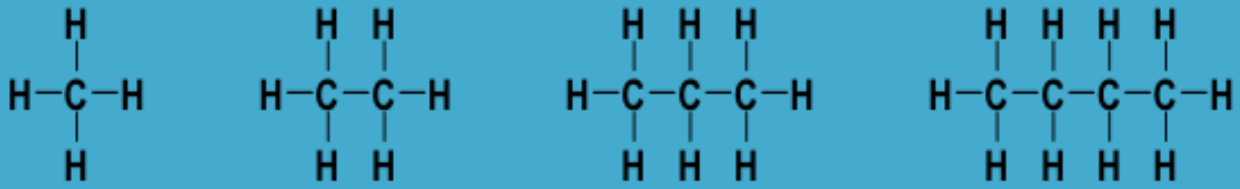
ALKANES

Table 12.2 Writing Structural Formulas for Some Alkanes

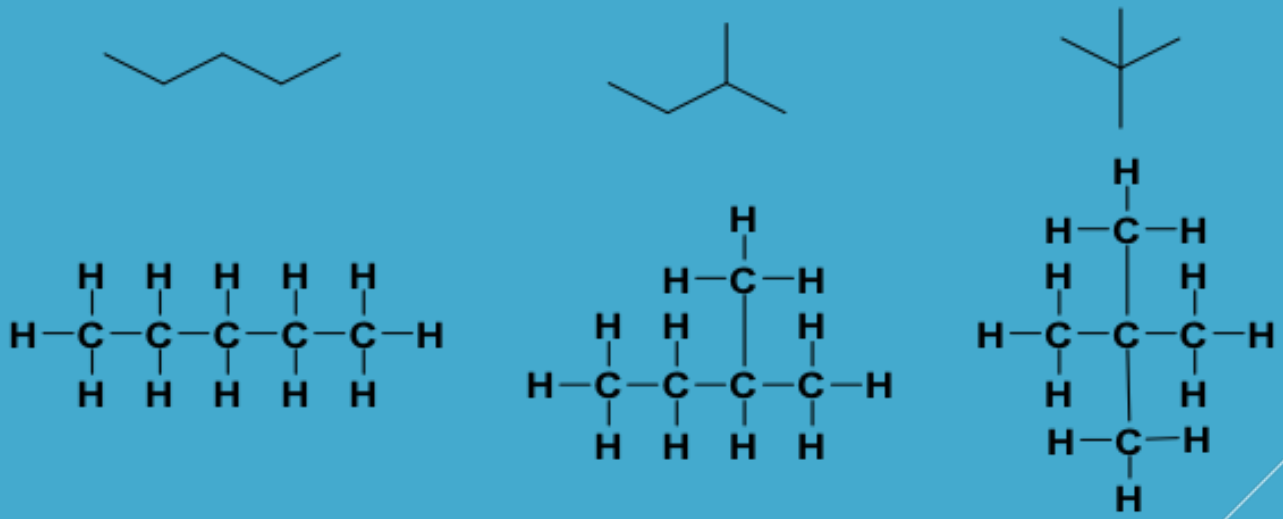
Alkane	Methane	Ethane	Propane
Molecular formula	CH_4	C_2H_6	C_3H_8
Structural formulas			
Expanded			
Condensed	CH_4	$CH_3—CH_3$	$CH_3—CH_2—CH_3$ or 
Line-bond			

NORMAL ALKANES AND BRANCHED ALKANES

Normal alkanes or straight-chain alkanes



Branched-chain alkanes

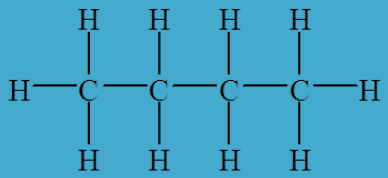


ISOMERS

Constitutional isomers

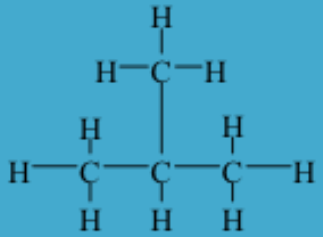
- Isomers that differ in how their atoms are arranged in chains are called **constitutional isomers.**
- **Isomers** have the same numbers and kinds of atoms but differ in the way the atoms are arranged.
- Compound like *n*-butane and isobutane, whose atoms are connected differently, are called constitutional isomers.
- Butane has 2 isomers: n-butane and isobutane.

n- butane



isobutane (or)

(2-methyl propane)



ISOMERS

Write the isomers of pentane(C5H10)?

CH3CH2CH2CH2CH3

ISOMERS:

1. Write the isomers of hexane C6H14?

CH3CH2CH2CH2CH2CH3

2. Write the isomers of heptane C7H16?

CH3CH2CH2CH2CH2CH2CH3

NAMES OF STRAIGHT-CHAIN ALKANES

Alkane	Name	Isomers
CH4	methane	1
C2H6	ethane	1
C3H8	propane	1
C4H10	butanes	2
C5H12	pentanes	3
C6H14	hexanes	5
C7H16	heptanes	9
C8H18	octanes	18
C9H20	nonanes	35
C10H22	decanes	75

ALKYL GROUPS

methyl: -CH3

ethyl: -C2H5 or -CH2CH3

propyl: -C3H7 or -CH2CH2CH3

butyl: -C4H9 or -CH2CH2CH2CH3

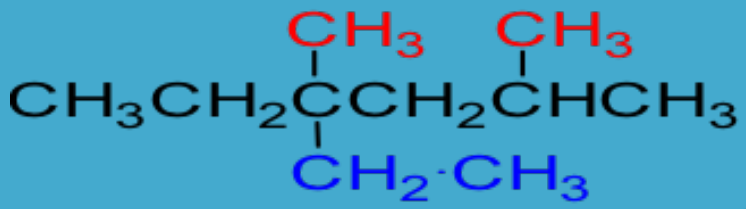
pentyl: -C5H11 or -CH2CH2CH2CH2CH3

Hexyl: - C6H13 or -CH2CH2CH2CH2CH2CH3 etc…..

Example :

4-ethyl

2,4-dimethyl



IUPAC NAME:

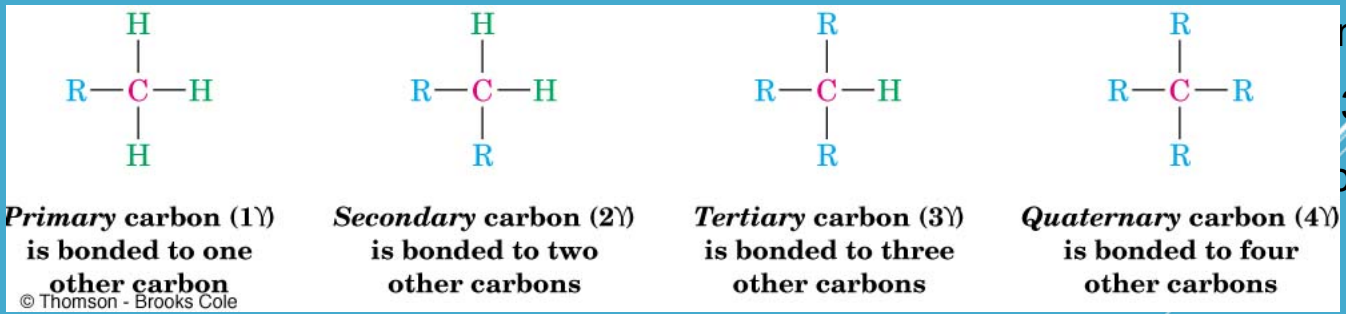
4-ethyl-2,4-dimethyl hexane

ALKYL GROUPS

Naming alkyl groups:

There are four types of alkyl groups ,depending on the number of other carbon atoms attached to the branched carbon atoms.

- A Carbon atom bonded to one carbon atom - Primary carbon(1˚).

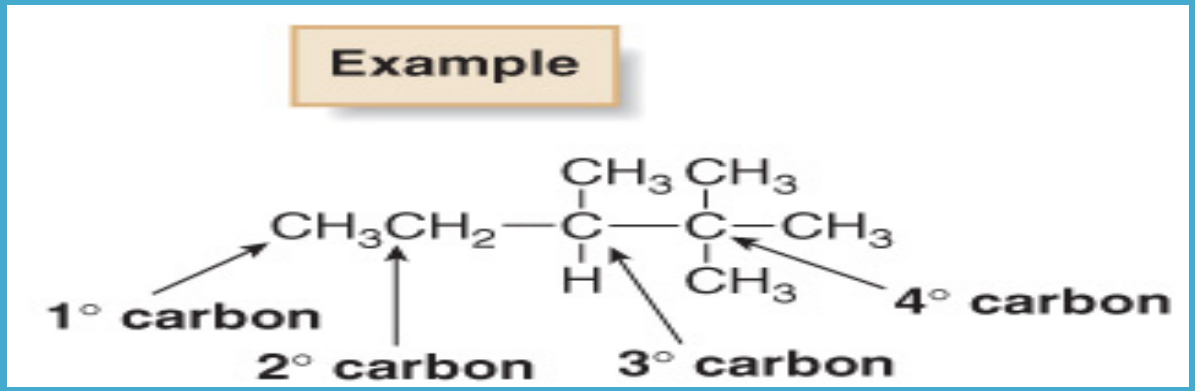


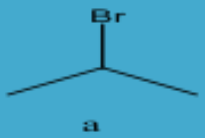
n(2˚).

3˚).

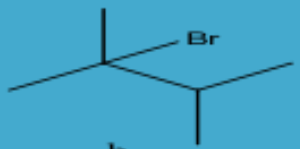
on(4˚).

EXAMPLE:



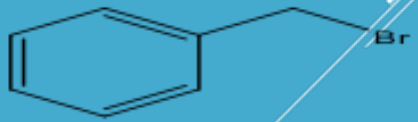


a



b

c

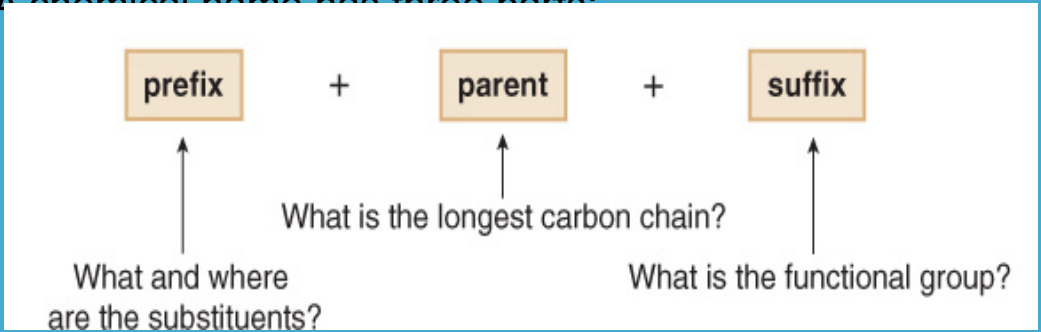


d

IUPAC NOMECLATURE

The system of naming organic compounds was devised by the International Union of Pure and Applied Chemistry(IUPAC)

A chemical name has three parts:

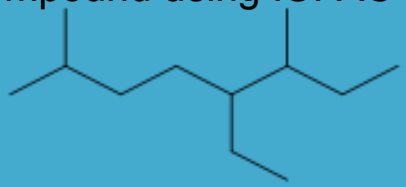


IUPAC rules for naming organic compound:

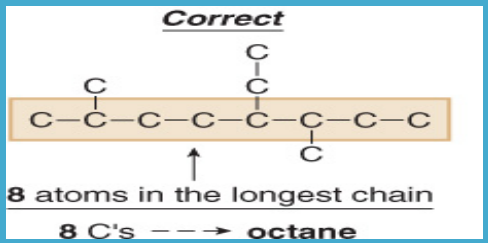
- Named as longest possible chain.
- Carbons in that chain are numbered in sequence.
- Substituents are numbered at their point of attachment.
- Lowest sum rule is applied for more than one substituent.
- Complex substituents are named as compounds.

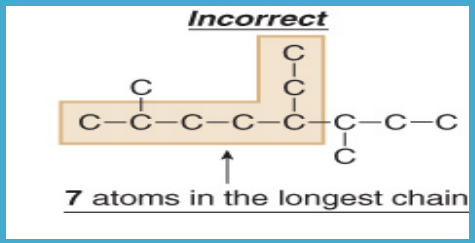
EXAMPLE

Name the organic compound using IUPAC nomenclature?



1. Identify the longest chain.



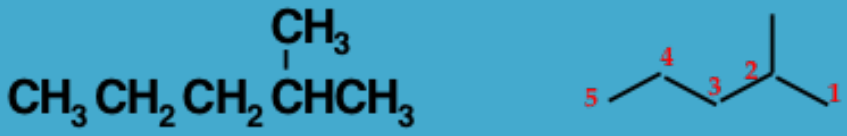


2. Identify the substituents attached to the longest chain with lowest sum rule. Two methyl groups at C-2 and C-6 ,ethyl group at C-5.

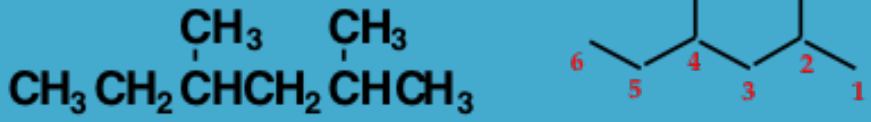
3. Find the position of the carbon atoms to which the substituent groups are bonded. In the presence of 2 or more substituents , Alphabetical order is followed.

IUPAC NAME OF THE COMPOUND IS- 5-ethyl-2,6-dimethyl octane.

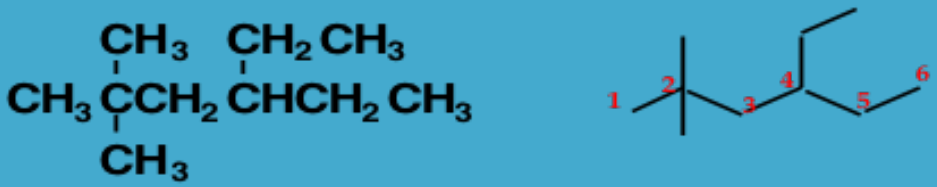
EXAMPLES

1. 

2-Methylpentane
(not 4-methylpentane)

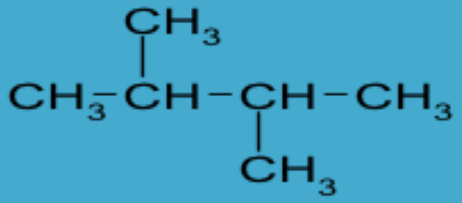
2. 

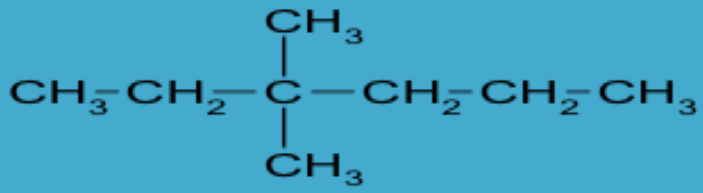
2,4-Dimethylhexane
(not 3,5-dimethylhexane)

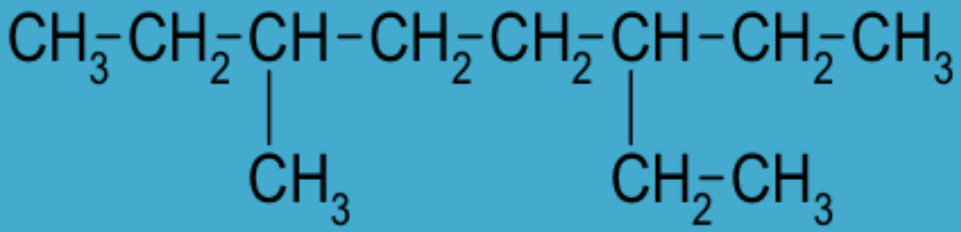
3. 

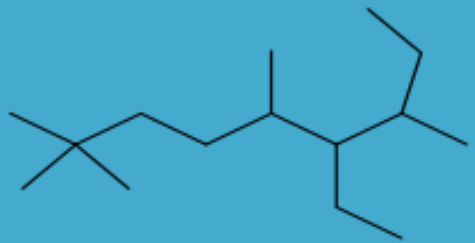
4-Ethyl-2,2-dimethylhexane
(not 2,2-dimethyl-4-ethylhexane)

PRACTICE PROBLEMS

1. 

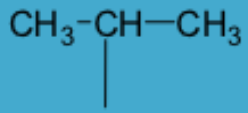
2. 

3. 

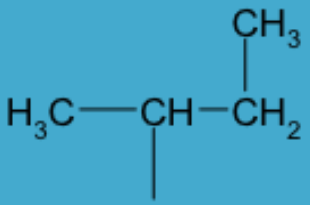
4. 

BRANCHED SUBSTITUENTS

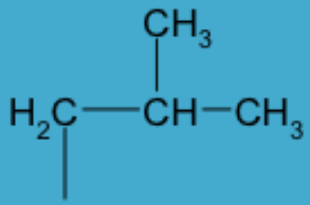
isopropyl (3 C-atoms)



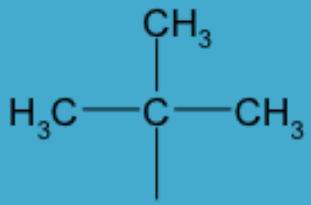
sec-butyl (4 C-atoms)



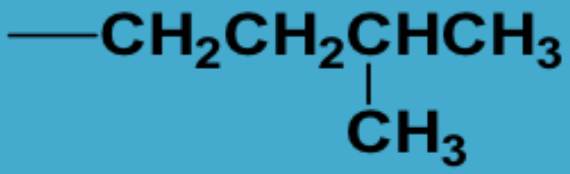
isobutyl



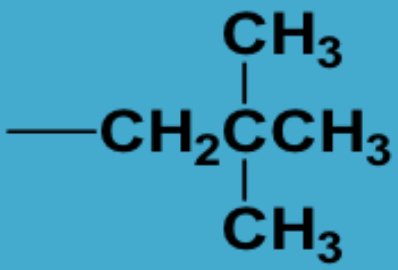
ter-butyl



isopentyl

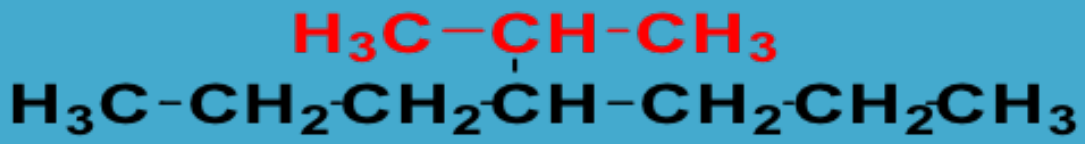


neo-pentyl (5 C-atoms)

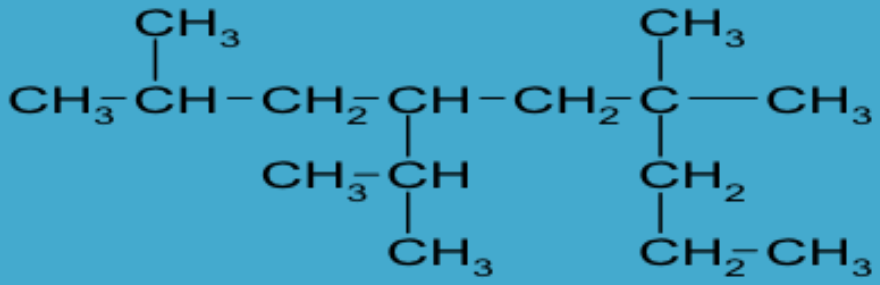


EXAMPLE

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



Find the IUPAC Name



NOMENCLATURE

Draw the structural formulas for the following compounds.

- 2-Methylheptane.
- 4-Isopropyl-3-methylheptane.
- 4-Ethyl-3,4-dimethyloctane.
- 2,4,4-Trimethylhexane.
- 4-Ethyl-2-methylhexane.
- 2,2,4-Trimethylpentane.
- 3-Isopropyl-2-methylhexane.

PHYSICAL PROPERTIES OF ALKANES

- They are also called **paraffins** because they do not react as most chemicals.
- The boiling point increases as they get more C-atoms in their formula.
- The melting point increases with an in increase in the molecular mass.
- Alkanes are non-polar so are immiscible with water, they are soluble in organic solvents.

Note: The dependence of the boiling and melting points on chain length can be explained in terms of increasing attractive van der Waals interactions as the chain length increases.

CHEMICAL PROPERTIES OF ALKANES

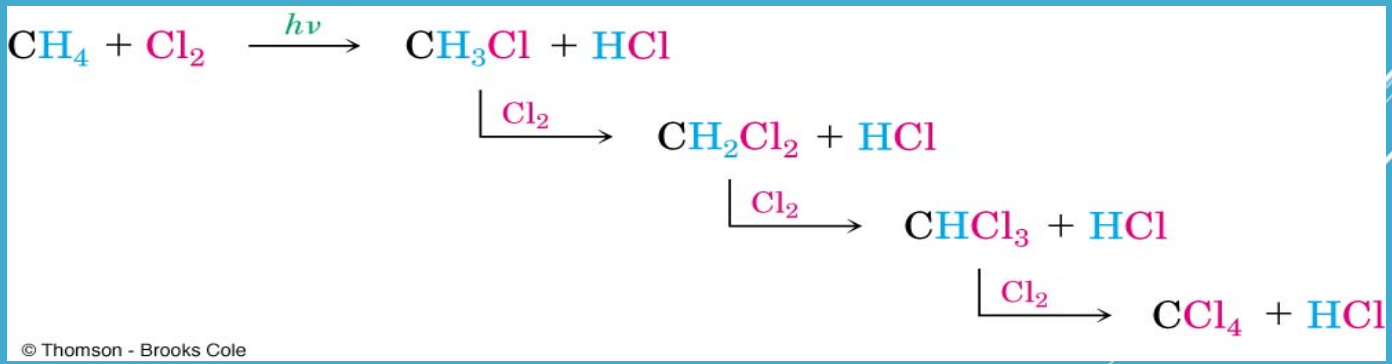
Combustion reaction:

Alkanes on complete combustion produce CO_2 , H_2O and large amount of heat is released.

$$CH_4 + 2O_2 \rightarrow CO_2 + H_2O + 890kJ/mol$$

Halogenation reaction:

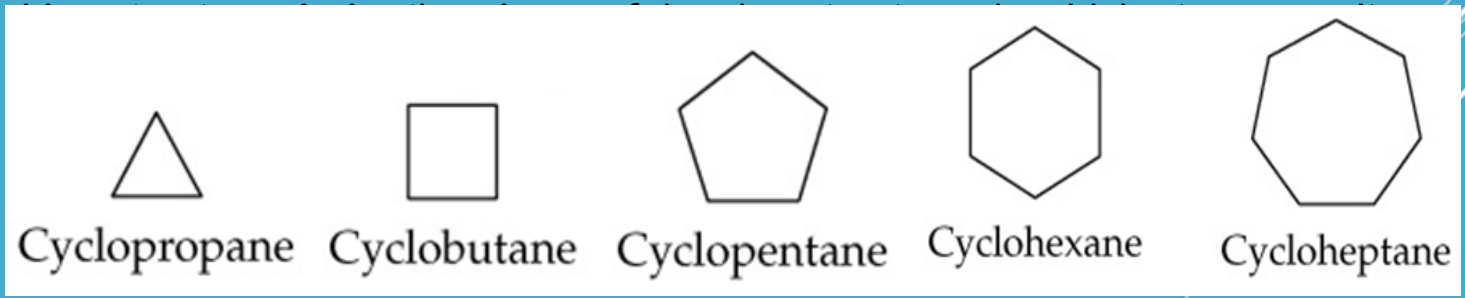
Alkanes react with chlorine in presence of sunlight leading to a mixtyre Of chlorinated products.



CYCLOALKANES

Cycloalkanes:

- An alkane that contains a ring of carbon atoms.
- Ring sizes from 3 carbons to 30 or higher are known.
- Cycloalkanes are represented by polygons.
- A triangle represents cyclopropane, a square represents cyclobutane, a pentagon represents cyclopentane, and so on.

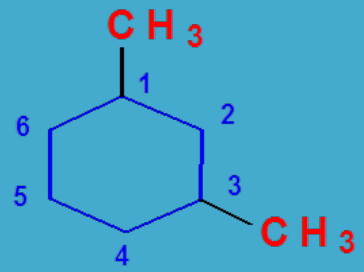


NOMENCLATURE OF CYCLOALKANES

- 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 cycloalkanes.
- 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.
- Number the substituents and write the name if only one substituent, no need to give it a number.

Example:

1,3-dimethylcyclohexane

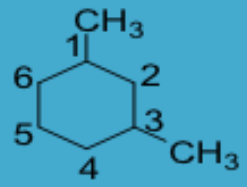


Note: Start at the point of attachment and number the substituents on the ring so as to arrive at the lowest sum.

EXAMPLES

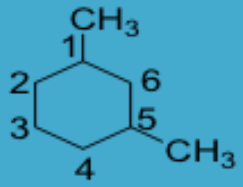
1.

Right



1,3-Dimethylcyclohexane

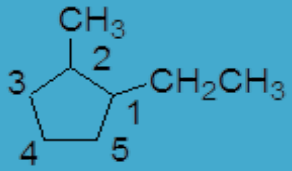
Wrong



1,5-Dimethylcyclohexane

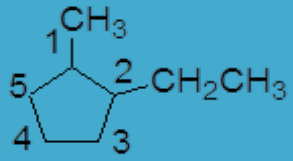
2.

Right



1-Ethyl-2-methylcyclopentane

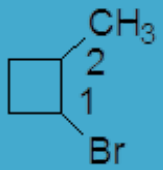
Wrong



2-Ethyl-1-methylcyclopentane

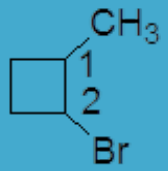
3.

Right



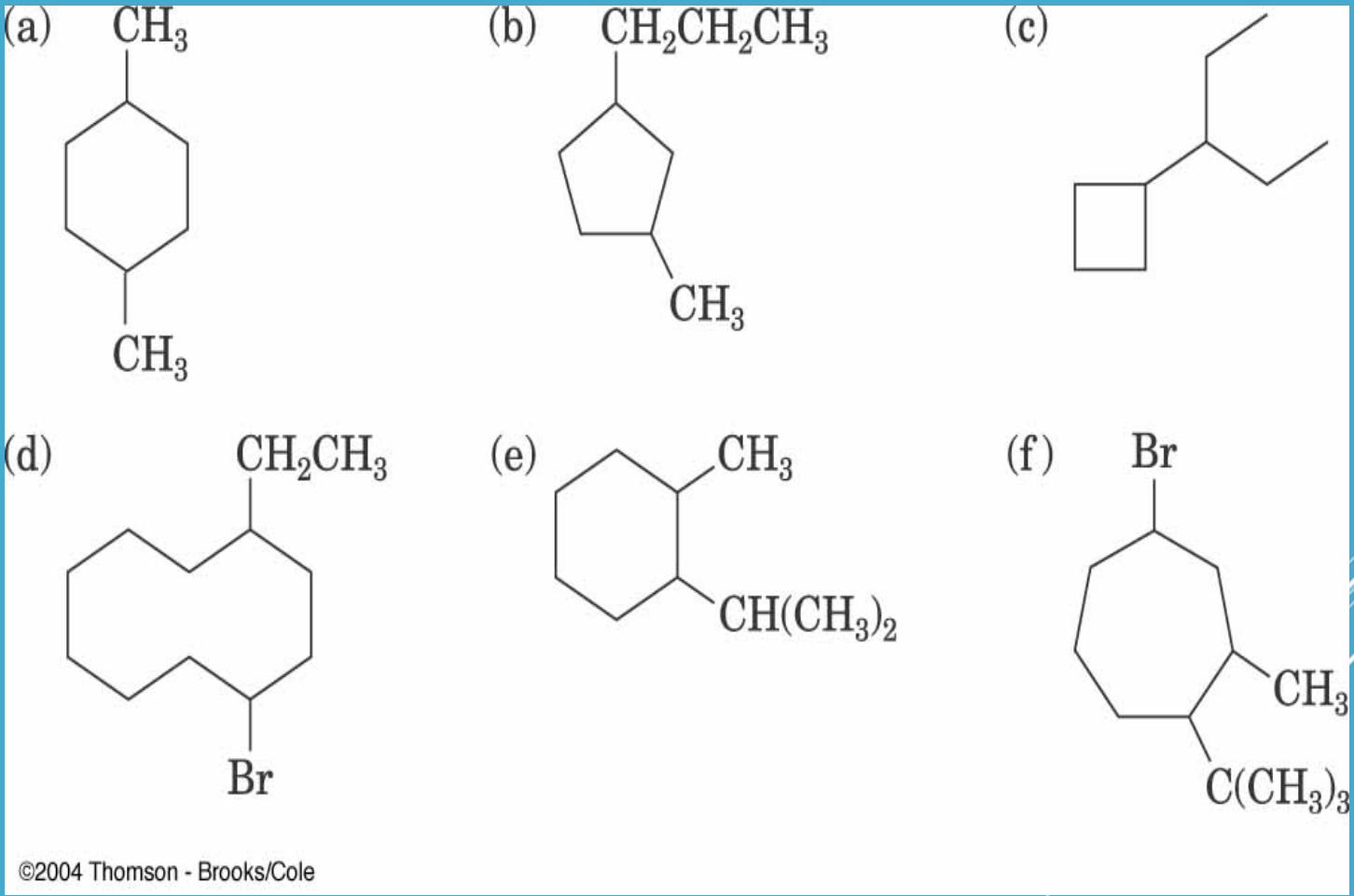
1-Bromo-2-methylcyclobutane

Wrong



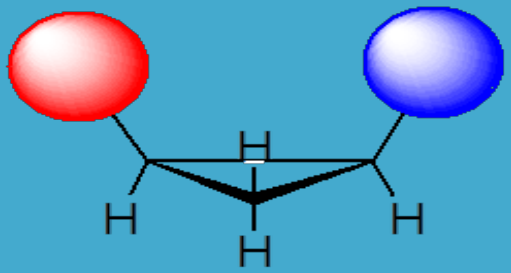
2-Bromo-1-methylcyclobutane

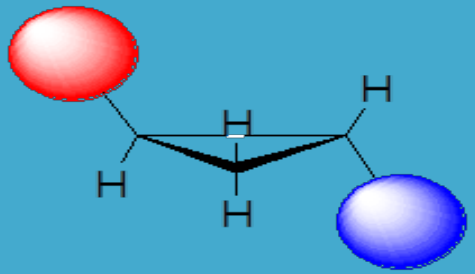
PRACTICE PROBLEMS

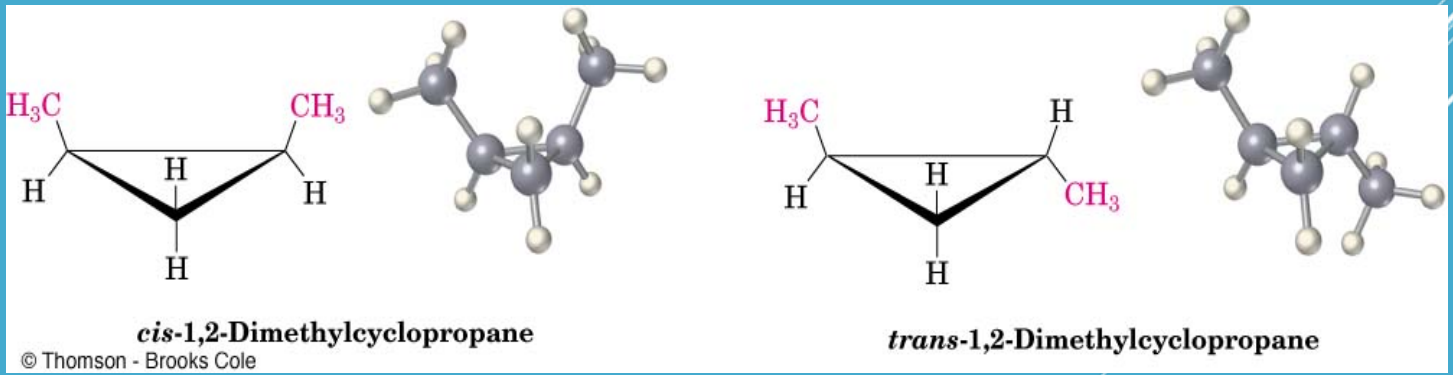


CIS-TRANS ISOMERISM

- Cycloalkane ring do not rotate freely in space.
- Cis Isomers are when two atoms are on the same side of a ring.
- Trans Isomers are when two atoms are on different side of a ring.

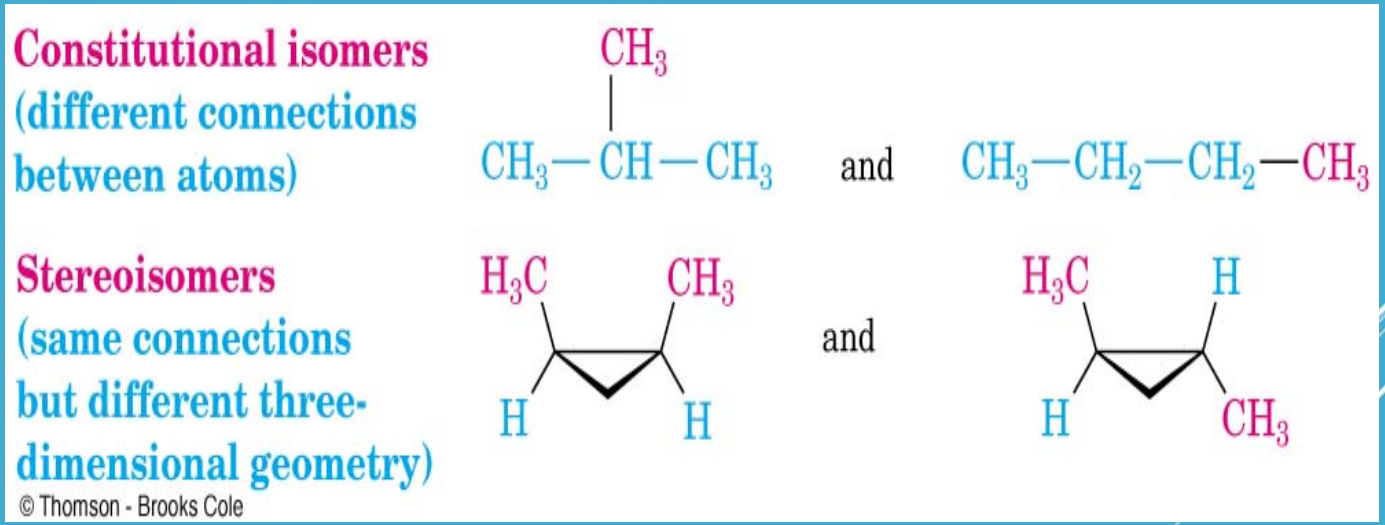




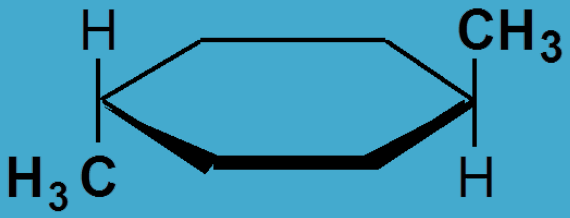


STEREOISOMERS

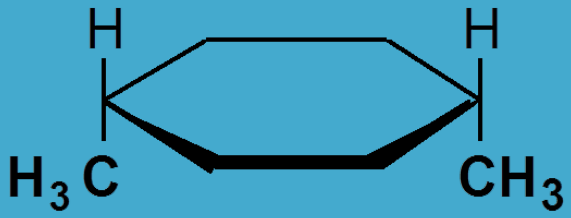
- Compounds with atoms connected in the same order but which differ in three-dimensional orientation, are **stereoisomers.**
- The terms “cis” and “trans” should be used to specify stereo isomeric ring structures.
- Recall that **constitutional isomers** have atoms connected in different order.



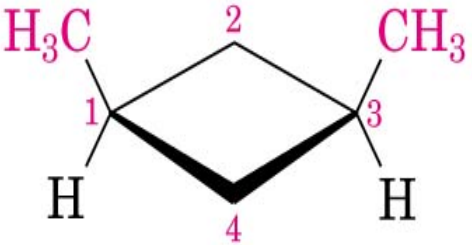
CIS-TRANS ISOMERS



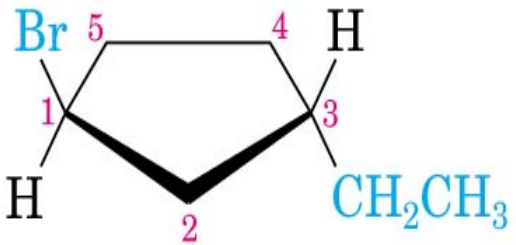
trans-1,4-Dimethyl-cyclohexane



cis-1,4-Dimethyl-cyclohexane

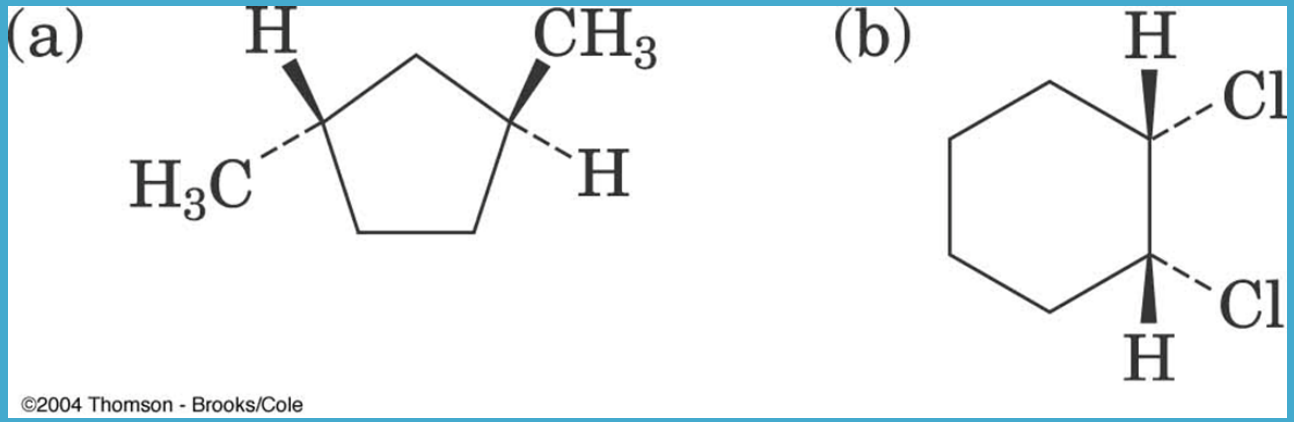


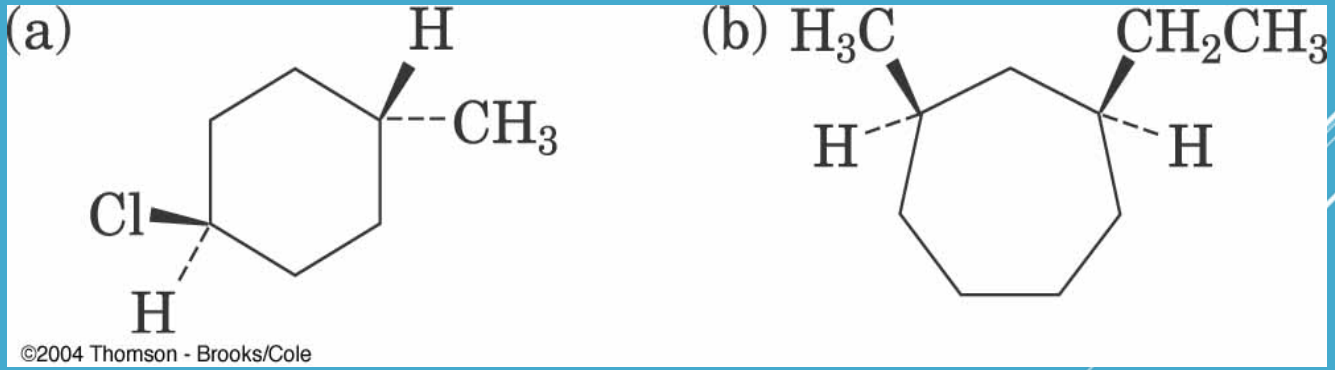
***cis*-1,3-Dimethylcyclobutane**



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

PRACTICE PROBLEMS

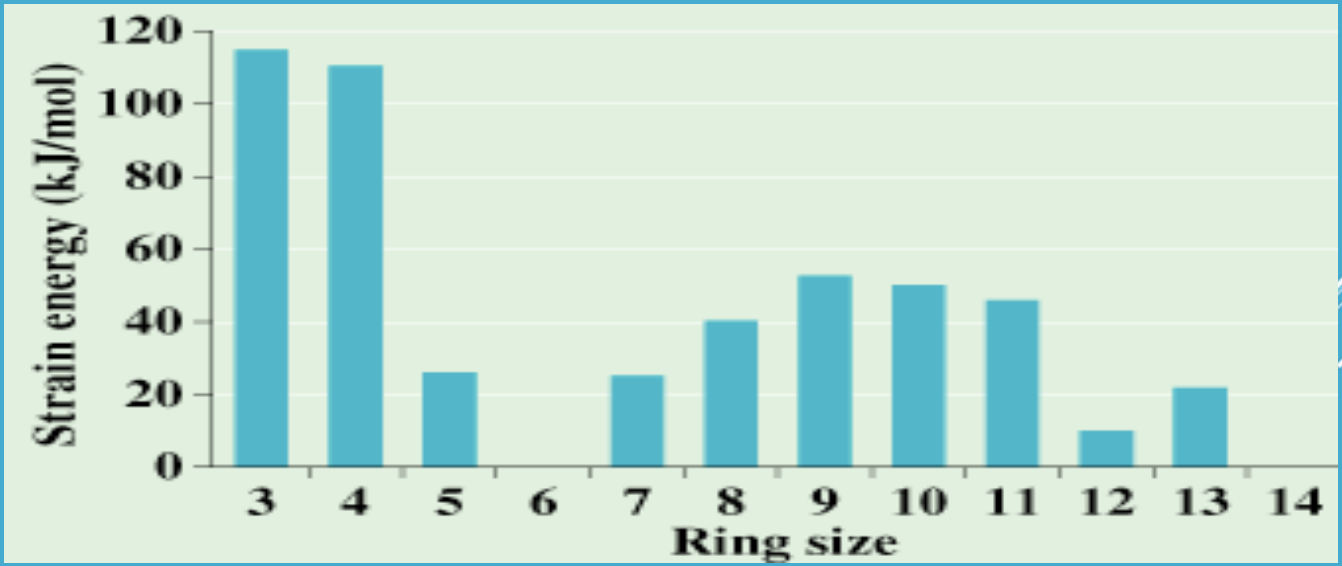




STEREOCHEMISTRY OF CYCLOALKANES

Baeyer (1885): since (sp3) carbon prefers to have bond angles of approximately 109°, ring sizes other than five and six may be too *strained* to exist.

Rings from 3 to 30 C's do exist but are strained due to bond bending distortions and steric interactions.

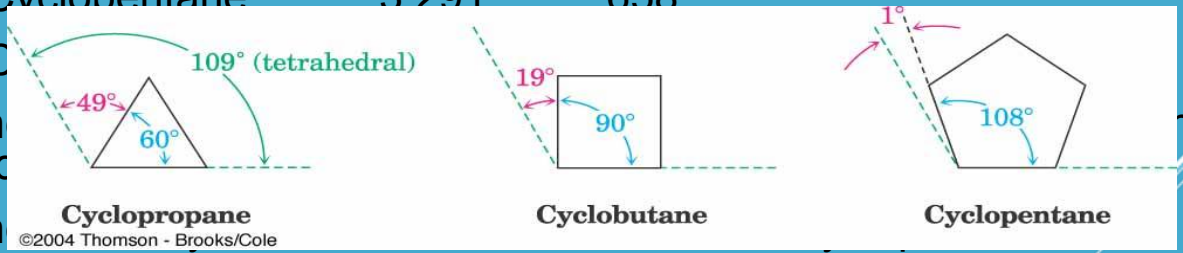


BAEYER'S STRAIN THEORY

- According to Baeyer, cyclopentane should have less angle strain than cyclohexane.

Cycloalkane	kJ/mol	Per CH2
Cyclopentane	3,291	658
C		

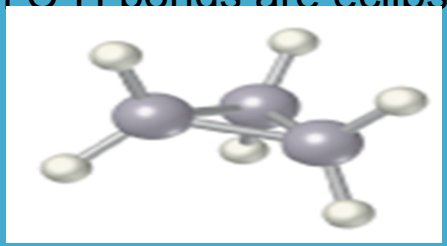
- Th… …han for cyc…
- Th…

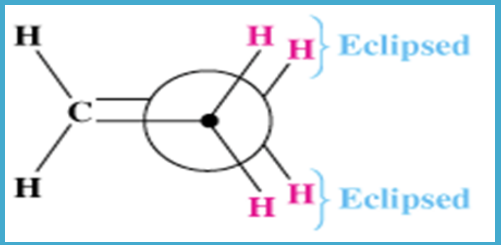


CONFORMATIONS OF CYCLOALKANES

Cyclopropane

- 3-membered ring must have planar structure.
- Symmetrical with C–C–C bond angles of 60°
- All C-H bonds are eclipsed.





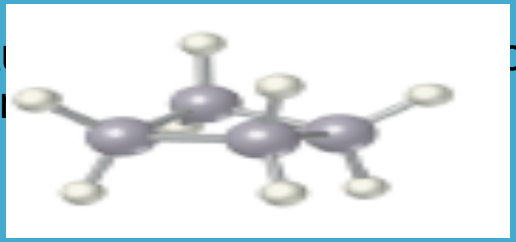
Cyclobutane

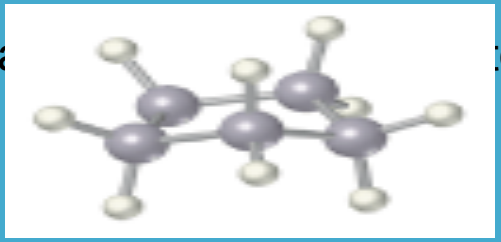
- Cyclobutane has less angle strain than cyclopropane but more torsional strain because of its larger number of ring hydrogen's.
- Cyclobutane is slightly bent out of plane.
- The bend *increases* angle strain but *decreases* torsional strain.

CONFORMATIONS OF CYCLOBUTANE AND CYLOPENTANE

Cyclopentane

- Planar cyclopentane would have no angle strain but very high torsional strain.
- Act[illegible]opentane a[illegible]orsional strai[illegible]





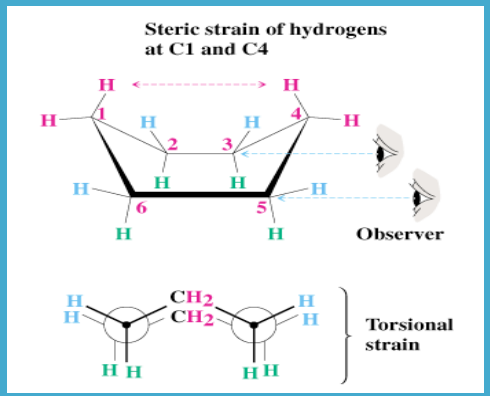
Actual conformations of cyclopentane are nonplanar, reducing torsional strain.

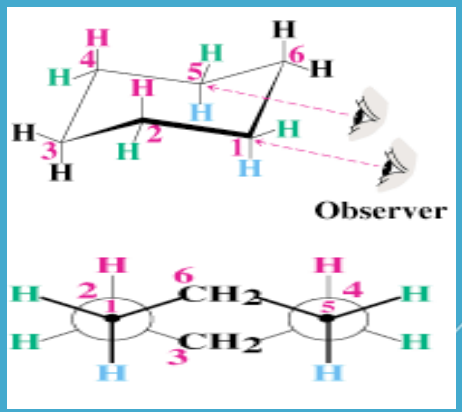
Cyclobutane

Cyclopentane

CONFORMATIONS OF CYCLOHEXANE

- Substituted cyclohexane occur widely in nature.
- Cyclohexane ring is not flat.
- The two conformations of cyclohexane are boat and chair form.
- But the chair form is more stable than boat form as, it has a puckered structure and strain-free 3-dimentional shape, with bond angles ideally close to 109.5□
- Chair form is more stable as it's free of angle strain and also torsional strain(neighboring C-H bonds are staggered).

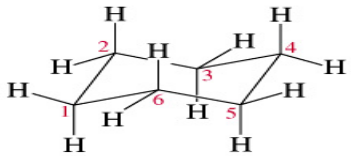




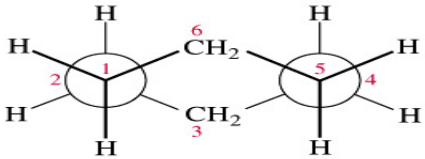
STABILITY OF CYCLOHEXANE

Chair is the most stable conformation of cyclohexane.

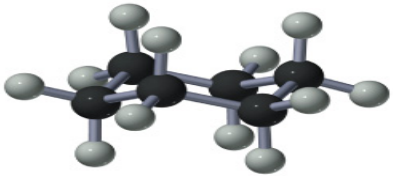
All of the bonds are staggered and the bond angles at carbon are close to tetrahedral.



chair conformer of cyclohexane



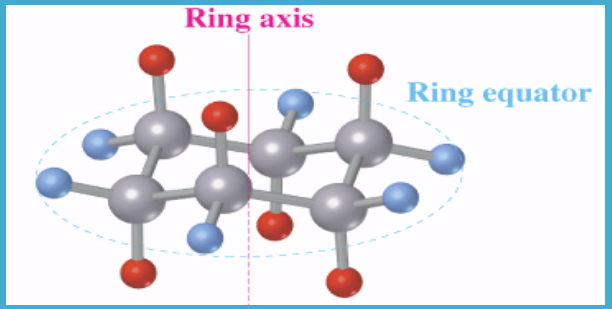
Newman projection of the chair conformer

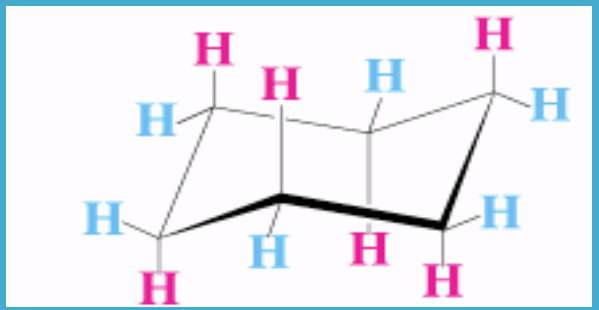


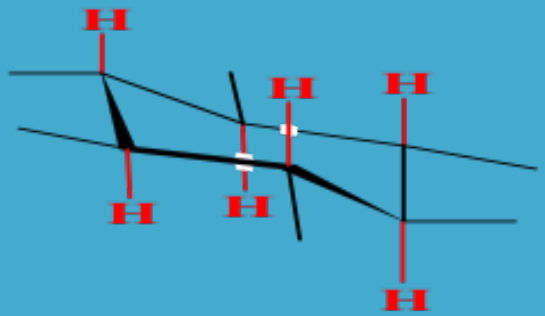
ball-and-stick model of the chair conformer of cyclohexane

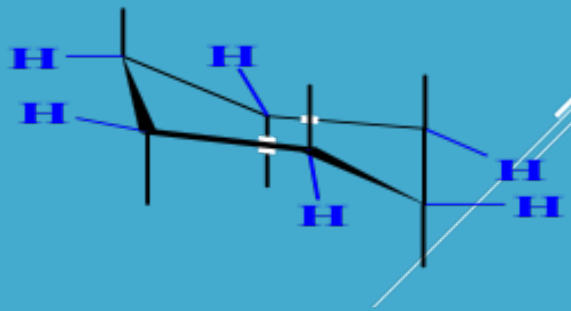
AXIAL AND EQUATORIAL BONDS IN CYCLOHEXANE

- The chair conformation has two kinds of positions for substituents on the ring: *axial* positions and *equatorial* positions.
- Chair cyclohexane has six **axial** hydrogens perpendicular to the ring (parallel to the ring axis) and six **equatorial** hydrogens near the plane of the ring .









CONFORMATIONAL MOBILITY OF CYCLOHEXANE

Chair conformations readily interconvert, resulting in the exchange of axial and equatorial positions by a **ring-flip.**

- **The chair conformation of cyclohexane is the most stable conformation and derivatives of cyclohexane almost always exist in the chair conformation.**