Chapter 3. An Introduction to Organic Compounds

Learning objectives:

1. Name alkanes, cycloalkanes, and alkyl halides.
2. Write the structures of constitutional (or structural) isomers of alkanes.
3. Draw Newman projections of alkanes in staggered and eclipsed conformations, and arrange the order of stability for these conformations (conformational isomers).
4. Identify *cis* and *trans* relationship for the substituents on cycloalkanes.
5. Draw chair conformation of cyclohexane with unambiguous representation of axial and equatorial substituents.
6. Complete the equilibrium of two chair conformational isomers for a substituted cyclohexane, indicate the change for the relative positions of axial and equatorial substituents, and reason the stability between these two isomers.
7. Know the classification of alkyl halides, alcohols, and amines.

Molecular model kit will be very helpful for learning the material in this chapter.

Sections to be covered (in the order of delivery):

3.1	How alkyl substituents are named
3.2	The nomenclature of alkanes
3.3	The nomenclature of cycloalkanes-skeletal structures
3.4	The nomenclature of alkyl halides
3.5	The classification of alkyl halides, alcohols, and amines
3.6	The structures of alkyl halides, alcohols, ethers, and amines
3.7	The physical properties of alkanes, alkyl halides, alcohols, ethers, and amines
3.8	Rotation occurs about carbon-carbon single bond
3.9	Some cycloalkanes have angle strain
3.10	Conformers of clcyohexane
3.11	Conformers of monosubstituted cyclohexanes
3.12	Conformers of disubstituted cyclohexanes
3.13	Fused cyclohexane rings

Recommended additional problems

35, 36, 38, 39, 40, 46, 52, 55, 61

3.1 How alkyl substituents are named

Alkyl groups are commonly represented as R.

methyl

ethyl

propyl (*n*-propyl)

isopropyl

butyl (*n*-butyl)

isobutyl

sec-butyl ((*s*-butyl)

tert-butyl (*t*-butyl)

3.2 The nomenclature of alkanes

General formula: C_nH_{2n+2}

A. Skeletal structures

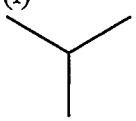
B. The IUPAC System (Systematic name) (in blue)

Important to know the names of alkanes from C = 1 to 10
Important to know the common alkyl groups

(i) Identify the longest carbon chain.
(ii) Locate the substituent with the lowest number on the parent (main) chain. If equivalent positions are encountered, assign the substituent with higher alphabetical order a higher priority (lower in numbering).
(iii) Place prefix of substituents according to their position on the main chain. Use di-, tri-, tetra-, penta-, hexa- and so on for identical substituents.
(iv) Arrange the substituents, excluding di-, tri-, tetra-, penta-, hexa- and so on, in alphabetical order.

Examples:

(i)



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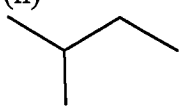

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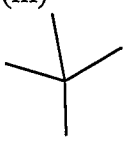

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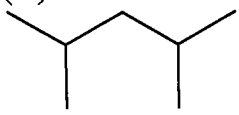

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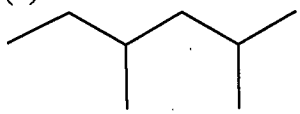

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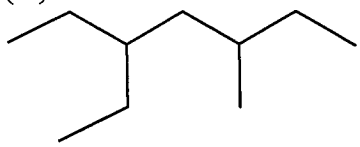

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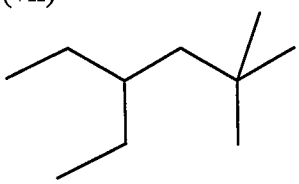

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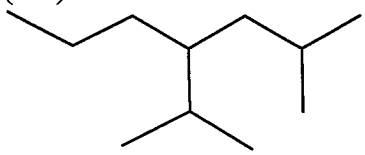

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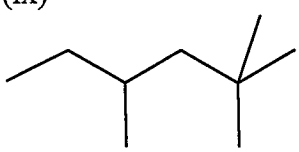

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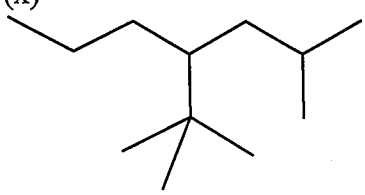

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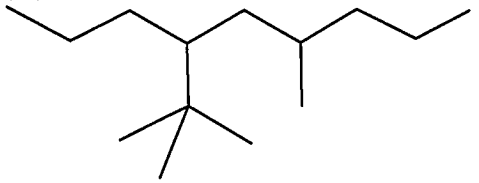


C. Structural isomers

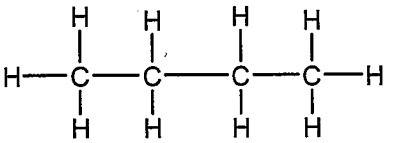
Structural (constitutional) isomers: Compounds with the same molecular formula but with different order of attachment (connectivity) of their atoms.

Examples:

(i) Butane (C_4H_{10})

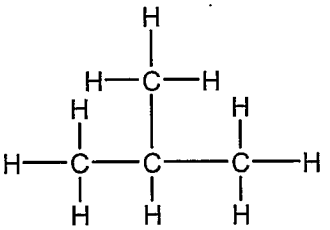
Normal butane (*n*-butane)

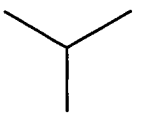
$CH_3CH_2CH_2CH_3$



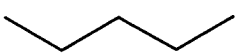
2-Methylpropane or isobutane (*iso*-butane or *i*-butane)

$CH_3CH(CH_3)CH_3$

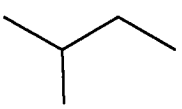




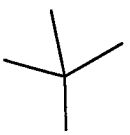
(ii) Pentane (C_5H_{12})



$CH_3CH_2CH_2CH_2CH_3$



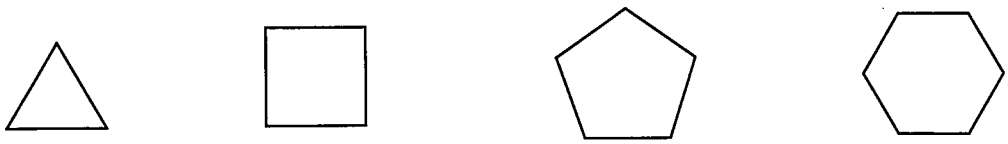
$CH_3CH(CH_3)CH_2CH_3$



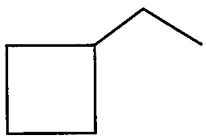
$CH_3C(CH_3)_2CH_3$

3.3 The nomenclature of cycloalkanes-skeletal structures

General formula: C_nH_{2n}



(i)



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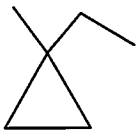

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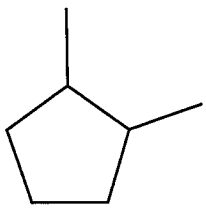

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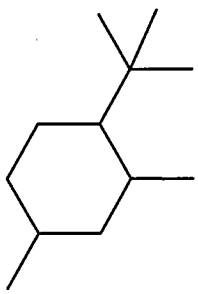

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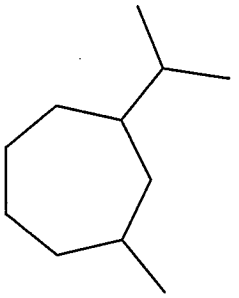


3.4 The nomenclature of alkyl halides

A. Systematic name (in blue)

Use the name of alkanes and treat halides as substituents.

B. Common Names (in red)

Use the name of alkyl groups.

Examples:

3.5 The classification of alkyl halides, alcohols, and amines

3.6 The structures of alkyl halides, alcohols, ethers, and amines

3.7 The physical properties of alkanes, alkyl halides, alcohols, ethers, and amines

Know induced-dipole-induced-dipole interaction (van der Waals interaction)

Know hydrogen bond

A. Boiling point

Boiling points of alkanes increase with increasing molecule weight.

B. Solubility in water

The presence of hydrogen bond or polar groups

C. Melting Point and Density

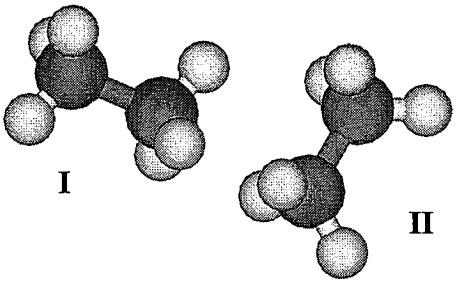
Melting points of alkanes are governed by the shape of molecule (packing of molecule) and molecule weight.

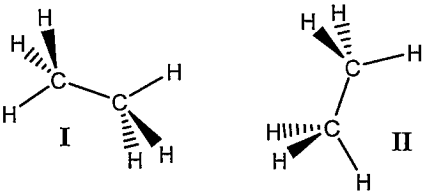
D. Constitutional Isomers Have Different Physical Properties

3.8 Rotation occurs about carbon-carbon single bond

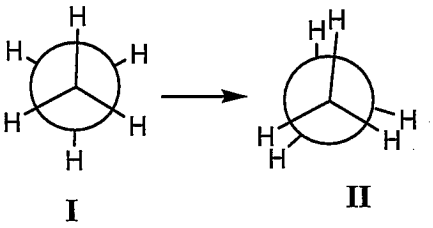
Conformation: result of single bond rotation

Conformational isomer: same atomic connectivity but different spatial arrangements of atoms.





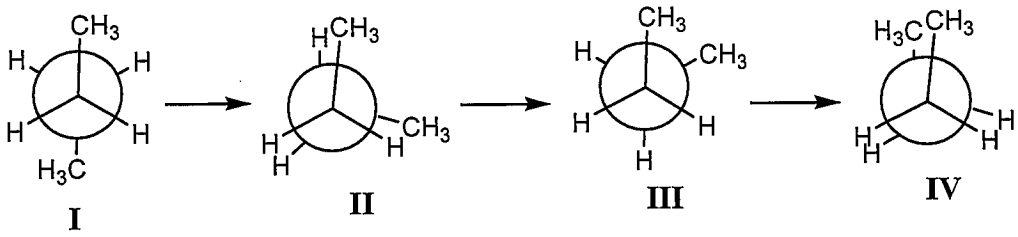
A. Newman projection of ethane



Staggered conformation

Eclipsed conformation

B. Newman projection of butane



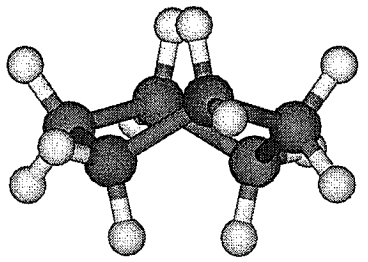
Steric strain (steric hindrance)

Anti-relationship

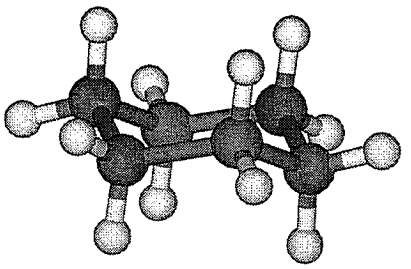
3.9 Some cycloalkanes have angle strain

3.10 Conformers of clcyohexane

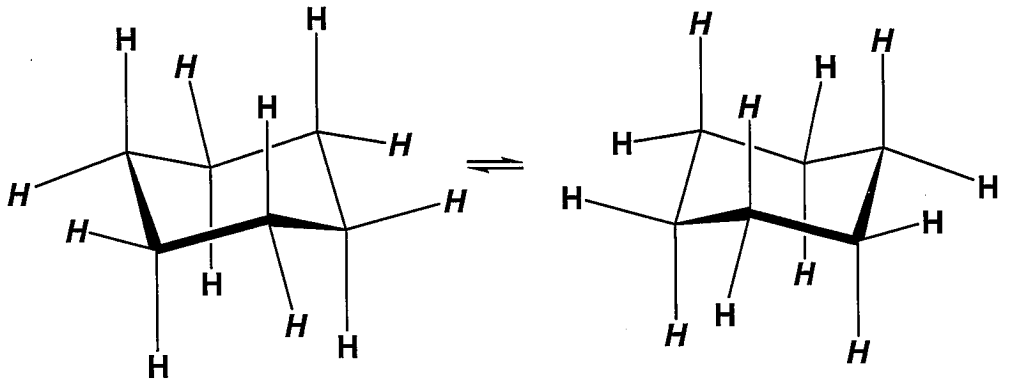
Know how to draw chair conformation of cyclohexane.
Know how to show axial and equatorial positions of cyclohexane.

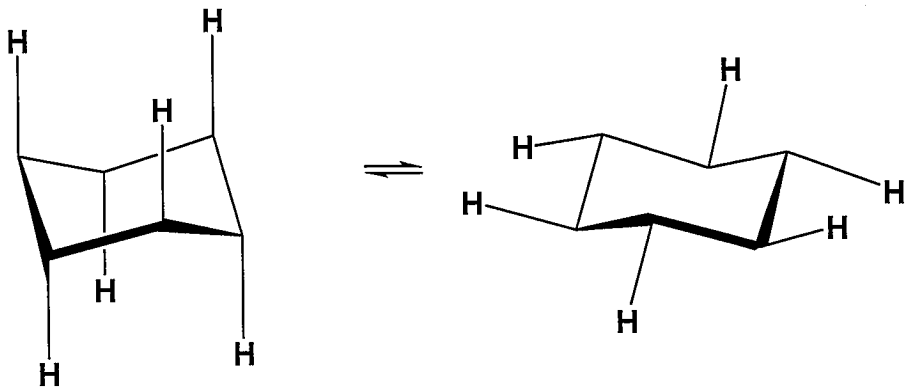


twisted



Chair

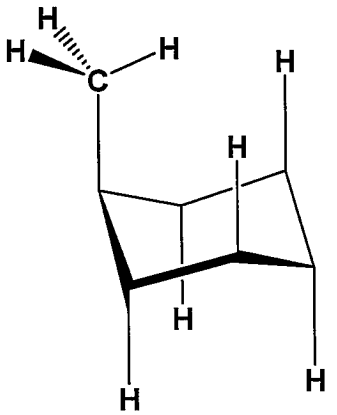


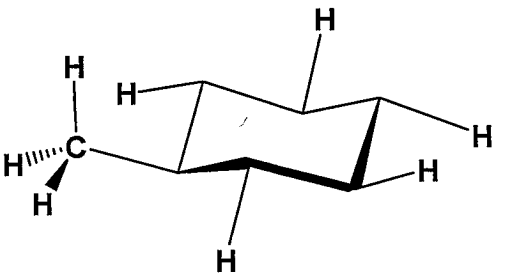


Equatorial position

Axial position

3.11 Conformers of monosubstituted cyclohexanes

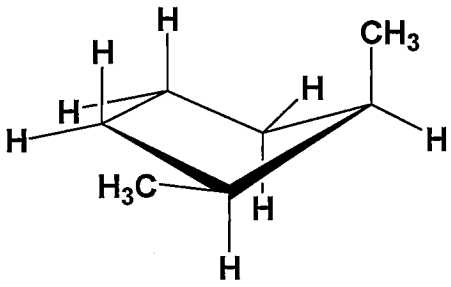


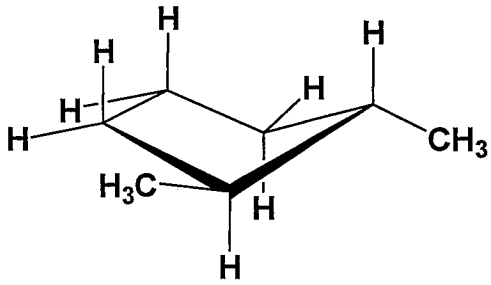


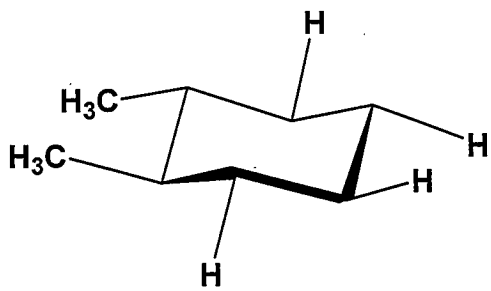
1,3-diaxial interaction (diaxial interaction, axial-axial interaction)

3.12 Conformers of disubstituted cyclohexanes

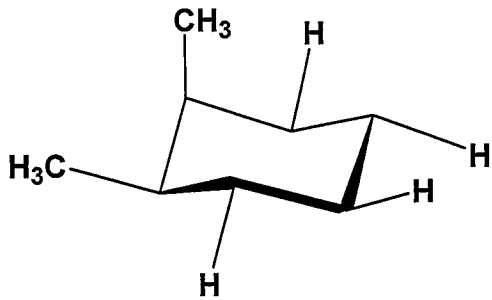
Know cis - trans isomerism in cycloalkanes





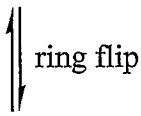


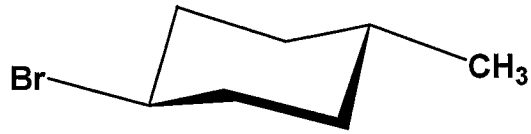
ring flip

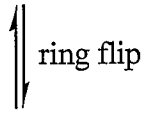


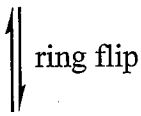
ring flip

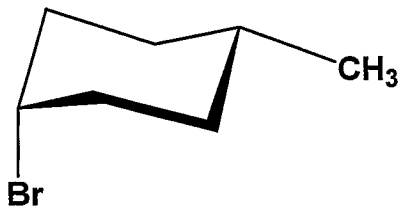
More examples:



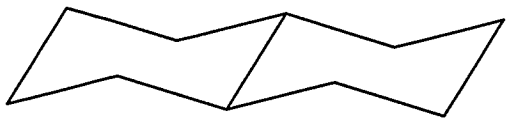




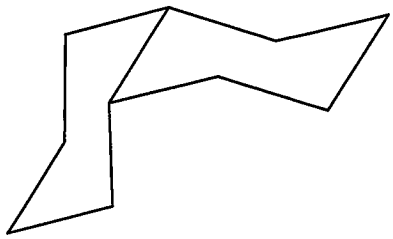




3.13 Fused cyclohexane rings



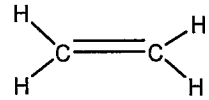
trans-fused rings



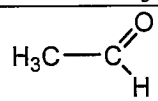
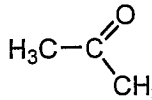
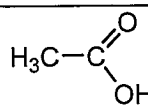
cis-fused rings

Additional information

Important infix

Infix	Nature of Carbon-carbon Bonds in the Main Chain	Example
-an-	All single (saturated) bond	H_3C-CH_3 Ethane
-en-	One or more double bonds	 Ethene (**ethylene**)
-yn-	One or more triple bonds	 Ethyne (**acetylene**)

Important suffix

Suffix	Class of Compound	Example
-e	hydrocarbon	$CH_3CH_2CH_2CH_2CH_3$ Pentane
-ol	alcohol	CH_3CH_2OH Ethanol
-al	aldehyde	 CH_3CHO acetaldehyde
-one	ketone	 CH_3COCH_3 acetone
-oic acid	carboxylic acid	 CH_3CO_2H acetic acid