

BIO-ORGANIC CHEMISTRY

(Organic Chemistry for Biology Students)

(SQBS 1603)

Alkanes

Dr Nik Ahmad Nizam Bin Nik Malek,

BSc (Ind. Chem.)(UTM), MSc (Chem)(UTM), PhD (Chem)(UTM), A.M.I.C

Senior Lecturer,

Department of Biotechnology and Medical Engineering

Faculty of Biosciences and Medical Engineering



The framework of organic compounds

- Hydrocarbon chain

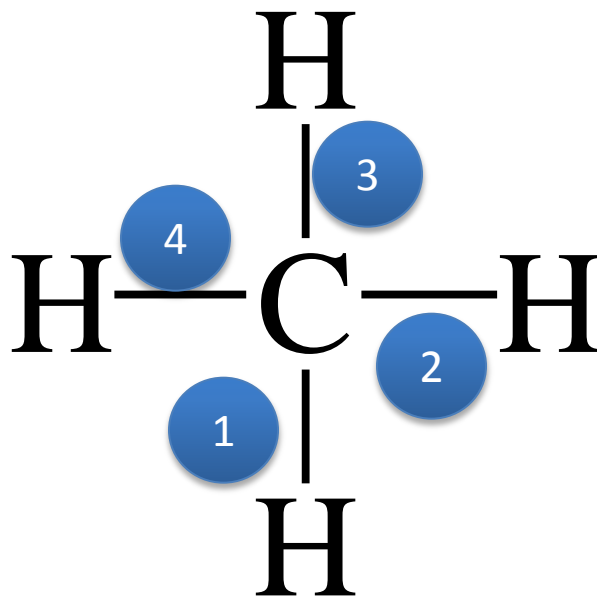
- H : Hydrogen
- C : Carbon
- Aliphatics
 - Alkanes
 - Alkenes
 - Alkynes
- Alicyclic
- aromatics

- Functional group

- Double bond (alkene)
- Triple bond (Alkyne)
- Amino (-NH₂)
- Benzene
- Phosphate (-PO₄)
- Carboxylic acids (-COOH)
- Alcohols (OH)
- Etc.

Hydrocarbon (HC)

- The simplest organic compounds comprise nothing more than a simple **carbon (C)** + **hydrogen (H)** skeleton, with no other functional groups attach.
- The simplest structure of HC is **methane**



Groups of Hydrocarbon

- **Alkane**
 - ❖ **Single** carbon-carbon bonds and no functional group
- **Alkene**
 - ❖ Contains at least one **double** carbon-carbon bonds as their functional group
- **Alkyne**
 - ❖ Contains at least one **triple** carbon-carbon bond as their functional group.
- **Aromatic HC**
 - ❖ Contains a benzene ring, a six membered ring with three double bonds.

Naming hydrocarbons

Two components

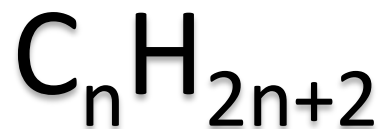
The **number of C** forming the longest unbroken chain in the molecule

Identifies the **hydrocarbon group** to which it belongs

1 st part	Number of C
Meth-	1
Eth-	2
Prop-	3
But-	4
Pent-	5
Hex-	6
Hept-	7
Oct-	8
Non	9
Dec-	10

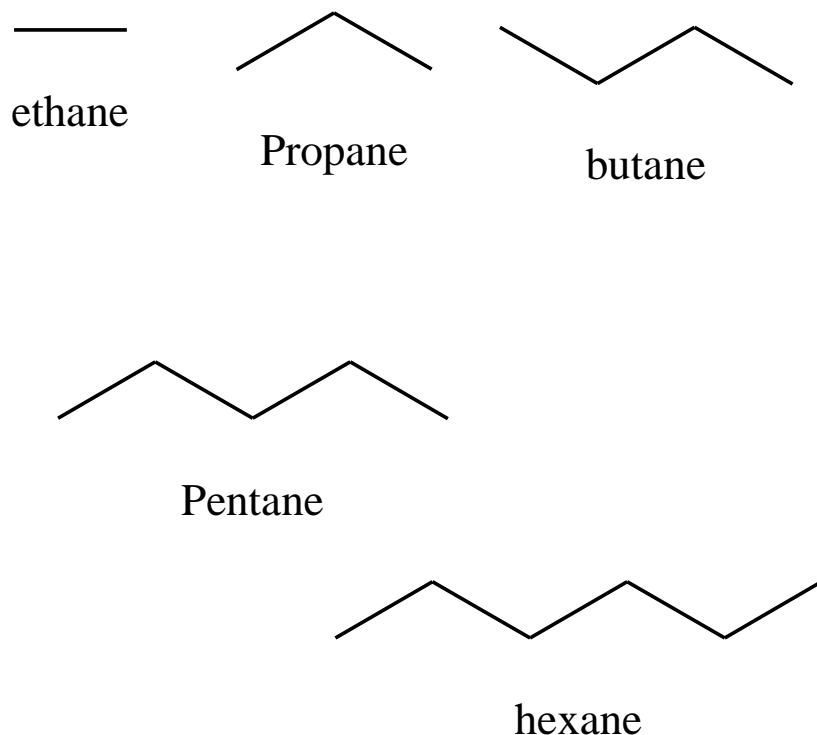
2 nd part	HC group
-ane	Alkane
-ene	Alkene
-yne	Alkyne

Homologous series of alkanes

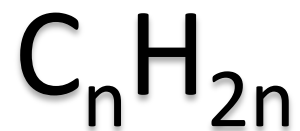


name	Number of C (n)	Molecular Formula
Methane	1	CH ₄
Ethane	2	C ₂ H ₆
Propane	3	C ₃ H ₈
Butane	4	C ₄ H ₁₀
Pentane	5	C ₅ H ₁₂
Hexane	6	C ₆ H ₁₄
Heptane	7	C ₇ H ₁₆
Octane	8	C ₈ H ₁₈
Nonane	9	C ₉ H ₂₀
Decane	10	C ₁₀ H ₂₂

Example of Skeletal Structural formula:

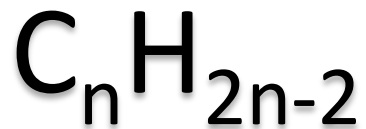


Homologous series of alkenes



name	Number of C (n)	Molecular Formula
Ethene	2	C_2H_4
Propene	3	C_3H_6
Butene	4	C_4H_8
Pentene	5	C_5H_{10}
Hexene	6	C_6H_{12}
Heptene	7	C_7H_{14}
Octene	8	C_8H_{16}
Nonene	9	C_9H_{18}
Decene	10	$C_{10}H_{20}$

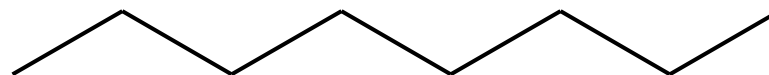
Homologous series of alkynes



name	Number of C (n)	Molecular Formula
Ethyne	2	C_2H_2
Propyne	3	C_3H_4
Butyne	4	C_4H_6
Pentyne	5	C_5H_8
Hexyne	6	C_6H_{10}
Heptyne	7	C_7H_{12}
Octyne	8	C_8H_{14}
Nonyne	9	C_9H_{16}
Decyne	10	$C_{10}H_{18}$

Alkanes

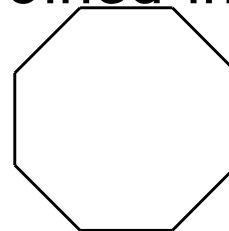
- Hydrocarbons having only C-C and C-H single bonds.
 - Acyclic or Aliphatic
 - Alkanes that contain **chains** of carbon atoms but **no rings**.



Octane

- Cycloalkanes

- Alkanes that contain carbons joined in one or more **rings**.

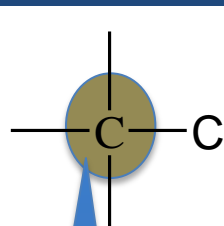


Cyclooctane

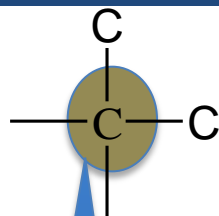
Simple alkanes

name	Number of C (n)	Molecular Formula
Methane	1	CH ₄
Ethane	2	C ₂ H ₆
Propane	3	C ₃ H ₈
Butane	4	C ₄ H ₁₀
Pentane	5	C ₅ H ₁₂
Hexane	6	C ₆ H ₁₄
Heptane	7	C ₇ H ₁₆
Octane	8	C ₈ H ₁₈
Nonane	9	C ₉ H ₂₀
Decane	10	C ₁₀ H ₂₂

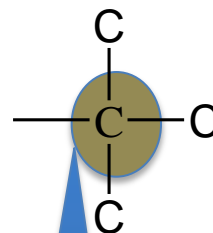
Classification of carbon atoms



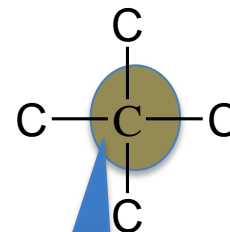
Primary
(1°)



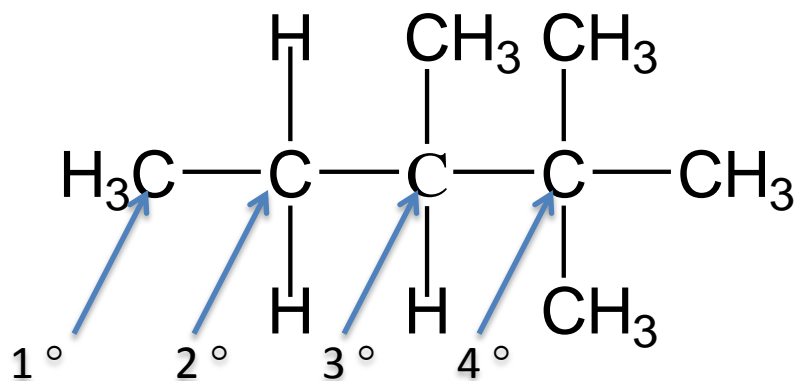
Secondary
(2°)



Tertiary
(3°)



Quaternary
(4°)

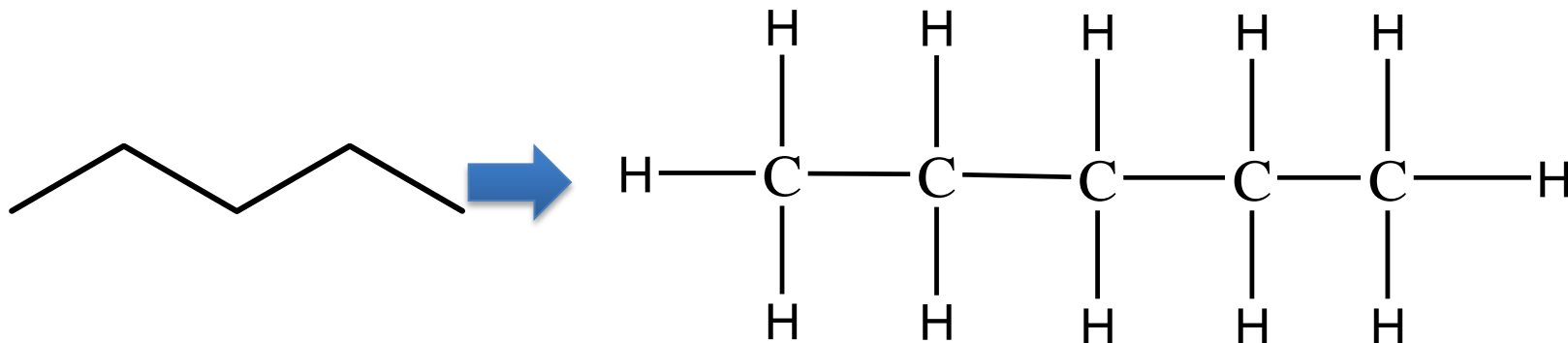


Nomenclature

Simple structure

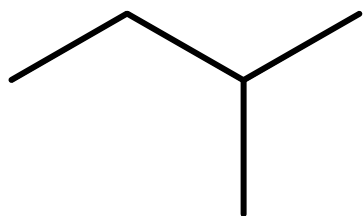
C → 5
H → 12
Single bond

C_5H_{12}
Pentane

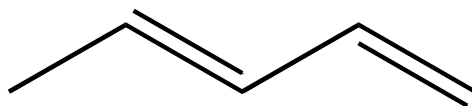


Nomenclature

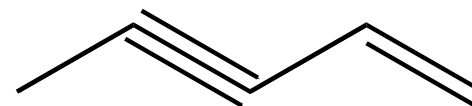
How about these
complicated structures?



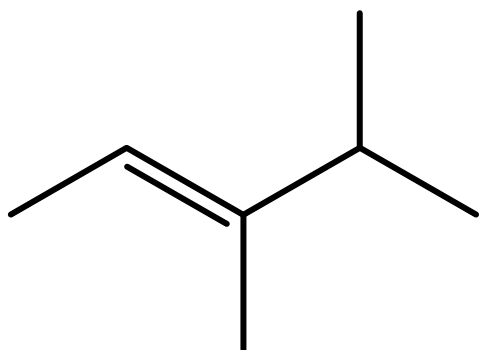
2-methyl-butane



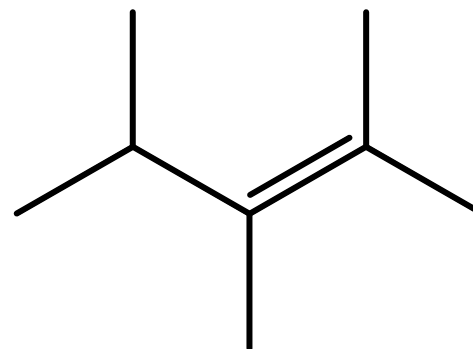
Penta-1,3-diene



Pent-1-en-3-yne



3,4-Dimethyl-pent-2-ene



2,3,4-Trimethyl-pent-2-ene

Nomenclature

Two names

**Common
names**

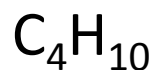
Not suitable to
name complicated
molecules

**IUPAC or Systematic
name**

IUPAC (International
Union of Pure and
Applied Chemistry)
rules

Nomenclature

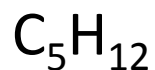
Common names



2 isomers

Butane

Isobutane



3 isomers

Pentane

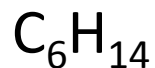
isopentane

neopentane

All of common names are based on historical names

Nomenclature

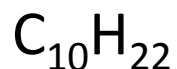
Problem with common names:



5 isomers



18 isomers

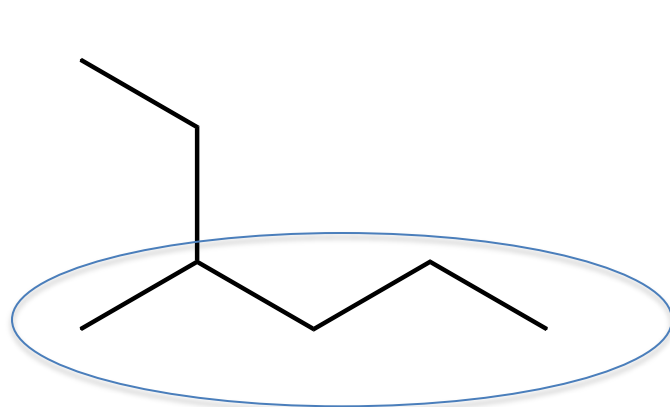


75 isomers

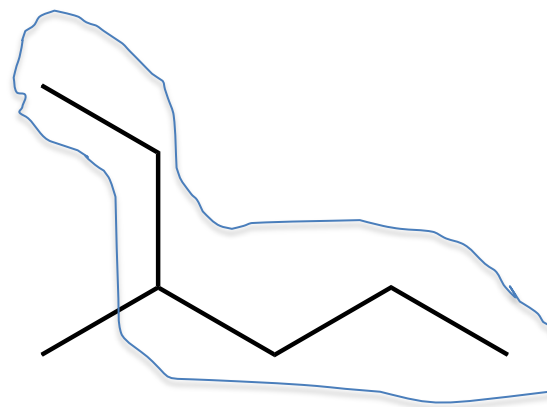
A systematic naming technique need to be applied when we want to name the organic compounds having complicated structure

Nomenclature

Base name → The longest continuous chain of C



C: 5



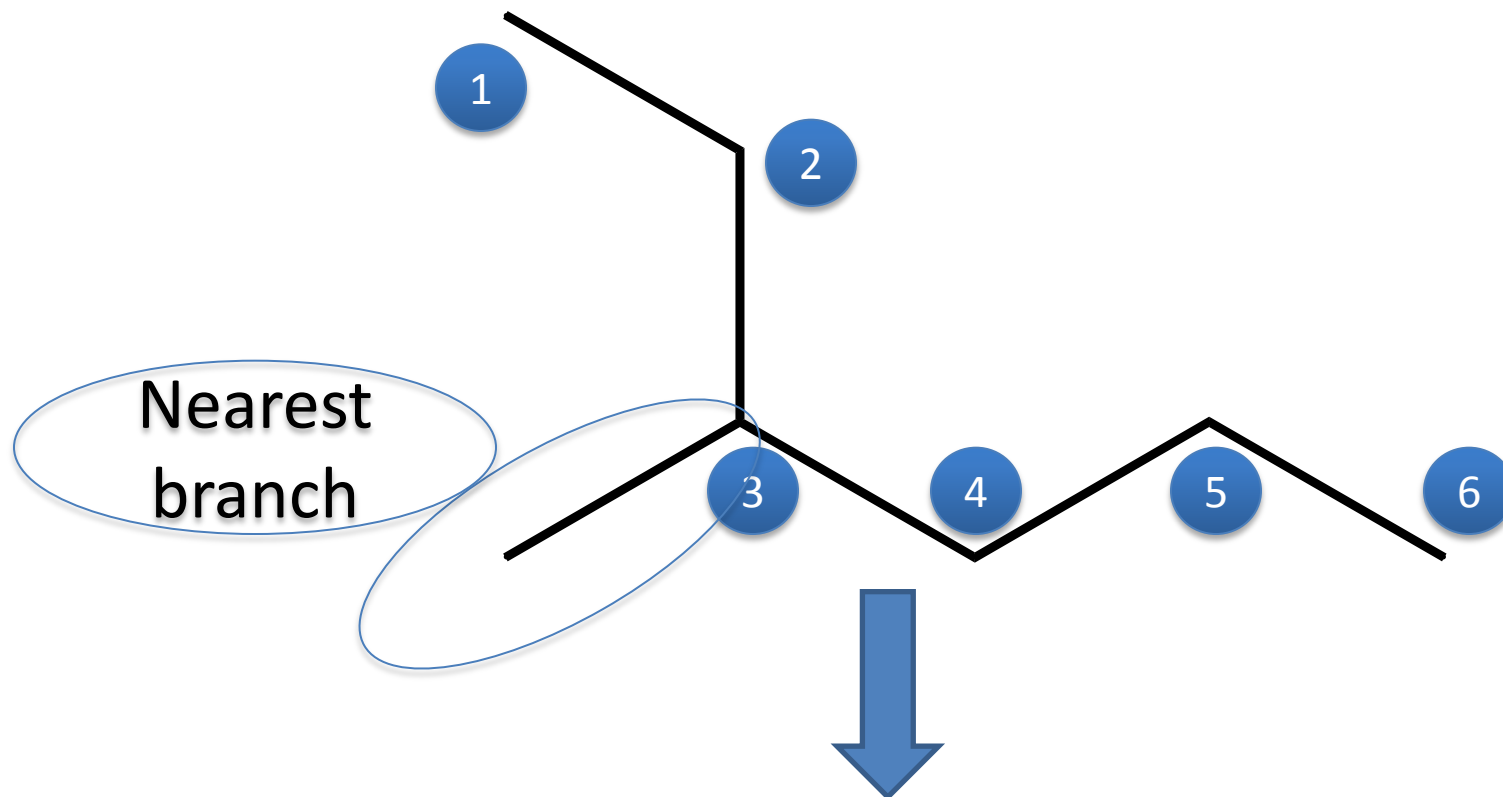
C: 6

hexane



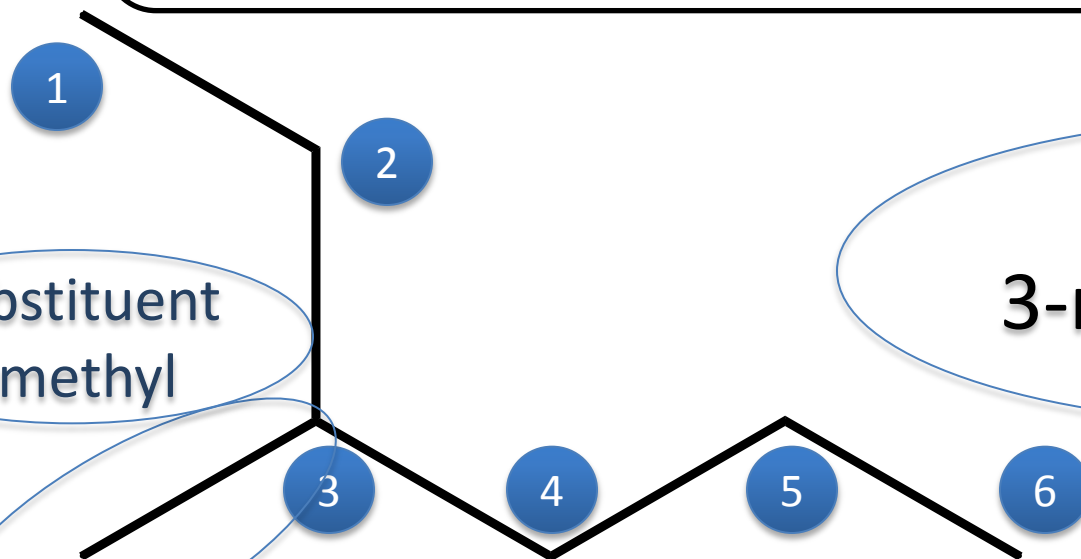
Nomenclature

Number the longest chain, beginning with the end nearest a branch



Nomenclature

Name the substituent on the longest chain (as alkyl groups). Give the locations of each substituent by the number of the main chain carbon atom to which it is attached



Substituent
: methyl

Location: 3

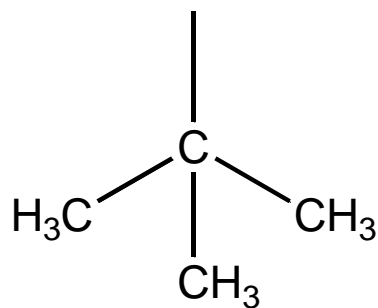
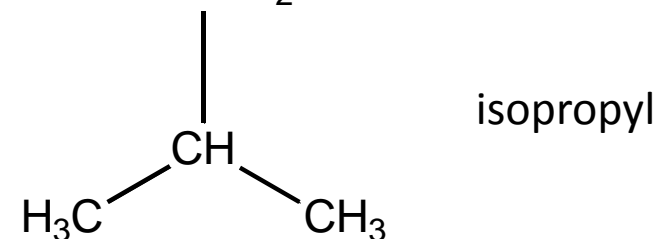
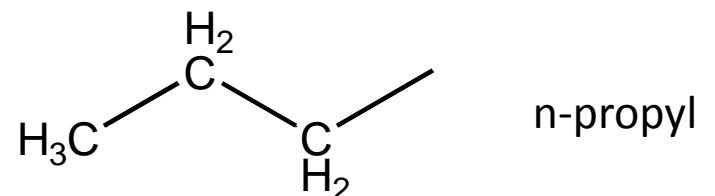
IUPAC name:

3-methylhexane

Nomenclature

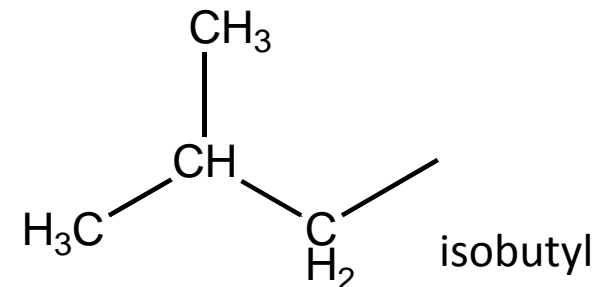
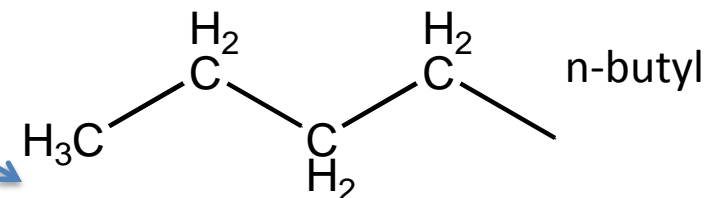
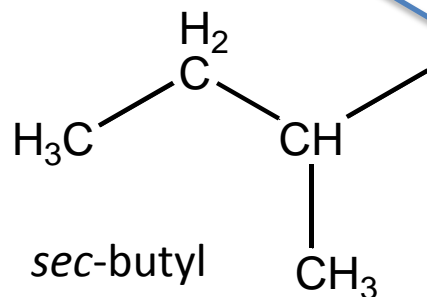
Substituent group

name	Number of C (n)	Molecular Formula
Methyl	1	CH ₃ -
Ethyl	2	C ₂ H ₅ -
Propyl	3	C ₃ H ₇ -
Butyl	4	C ₄ H ₉ -



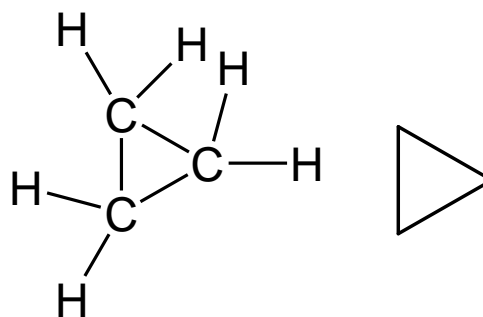
tert-butyl (*t*-butyl)

21

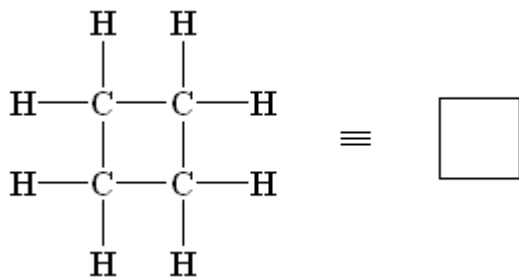


Cycloalkanes

- Carbon atoms arranged in a ring
- Examples:



Cyclopropane



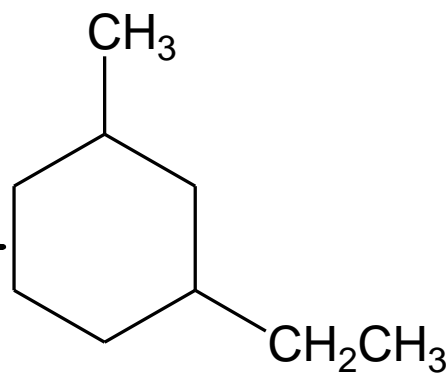
Cyclobutane

Nomenclature

1. Parent cycloalkane

- ❑ Count the number atoms in the ring.
- ❑ Use the parent name for that number of carbons.
- ❑ Add the prefix **cyclo-** and the suffix **-ane** to the parent name.

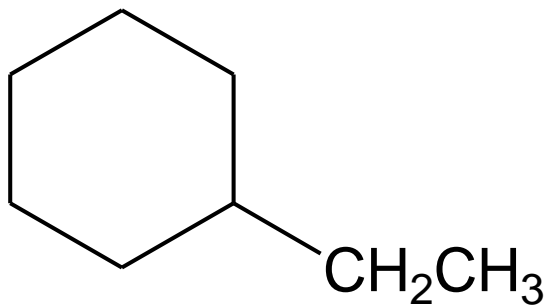
6 C's = hexane =
cyclohexane



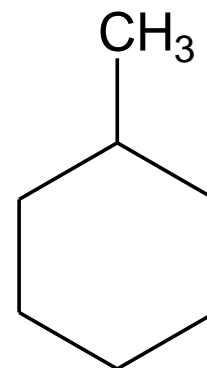
Nomenclature

2. Name and number the substituents

- No number is needed to indicate the location of a single substituents



Ethyl-cyclohexane



Methyl-cyclohexane

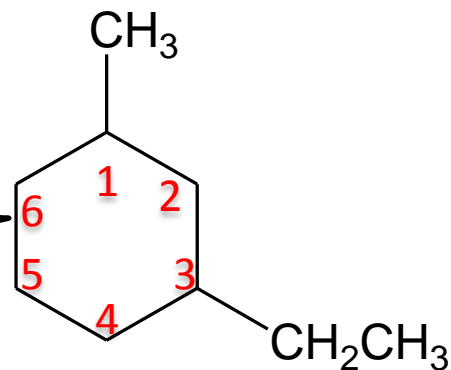
Nomenclature

2. Name and number the substituents

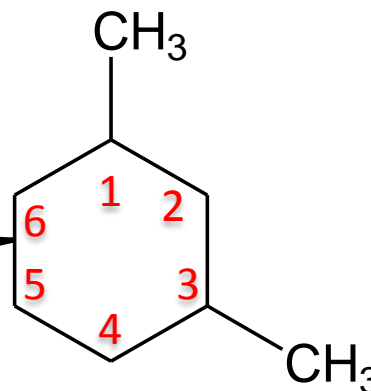
□ For rings than one substituents

- ❖ Begin numbering at one substituents,
- ❖ And then give the second substituents the lower number.

1-ethyl-3-methylcyclohexane
(not 3-ethyl-1-methylcyclohexane)

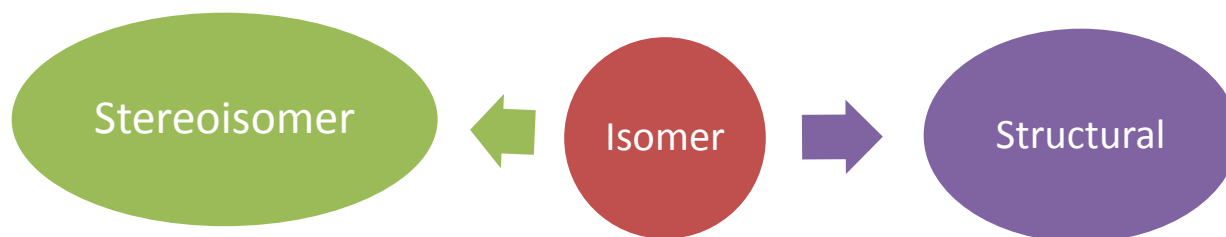


1,3-dimethylcyclohexane
(not 1,5-dimethylcyclohexane)



Isomers

- Groups of compounds that comprise exactly **the same atoms (same chemical composition) but which have different structure**, and often different physical and chemical properties too.

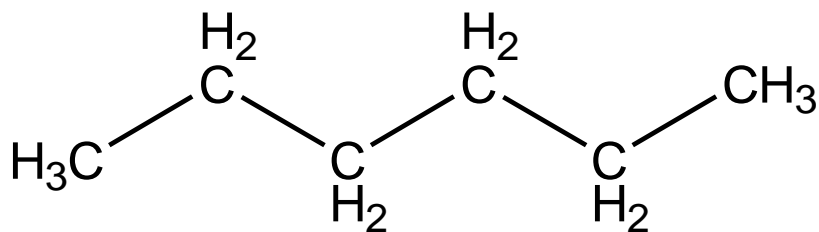


Structural Isomers

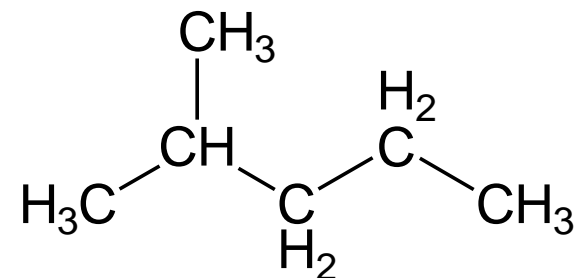
- Molecules that have the same chemical composition but the atoms are linked together in different ways.
- Compounds having similar **molecular formula** but with different **structural formula**.

Structural Isomers

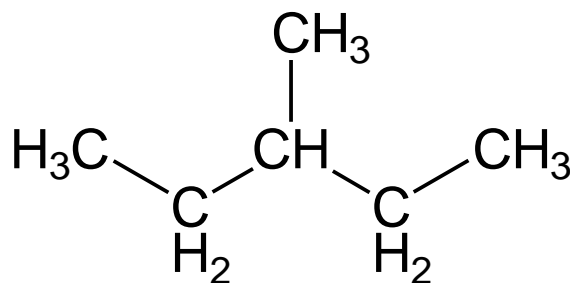
- structural isomers for compounds having molecular formula of C_6H_{14}



Hexane



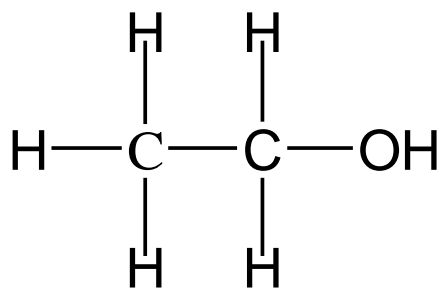
2-methylpentane



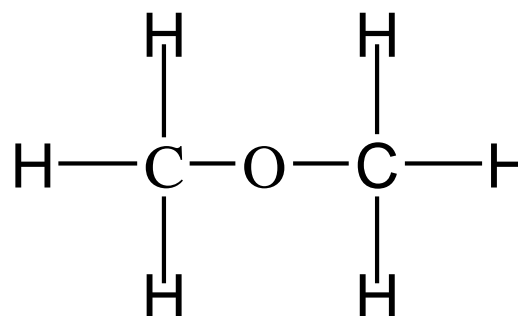
3-Methyl-pentane

Structural Isomers

- The important of structural formula
 - Can depicts how **the atoms are connected to one another** in the molecule.
 - E.g: C_2H_6O



Ethanol



Methoxymethane (dimethyl ether)

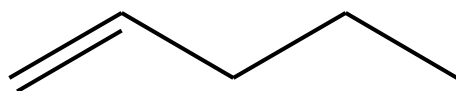
Structural Isomers

- The **shape of the carbon framework**
 - The number of different structural isomers that are possible increases dramatically as we consider alkanes with hydrocarbon chains of increasing length.

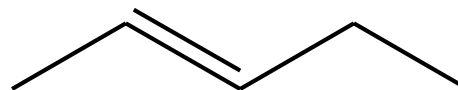
Number of C atoms in alkane	1-3	4	5	6	7	8	9	10	15	20
Number of possible structural isomers	1	2	3	5	9	18	35	75	4347	366319

Structural Isomers

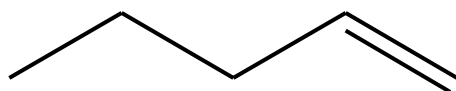
- The positioning of functional groups



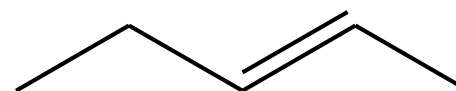
Pent-1-ene



Pent-2-ene



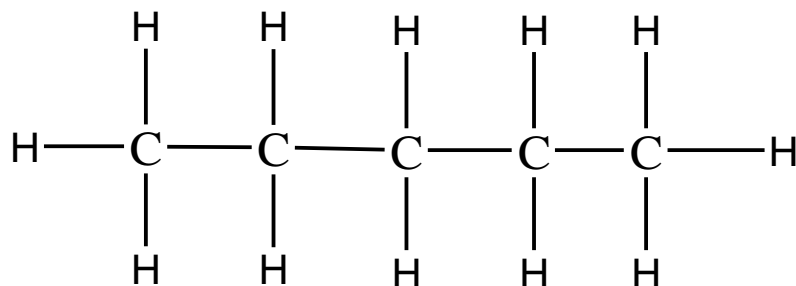
Pent-1-ene



Pent-2-ene

Molecular formula: C_5H_{10}

Physical properties of the alkanes



1) Non-polar

2) Lack the ability to form hydrogen bonding, dipolar or ionic interaction

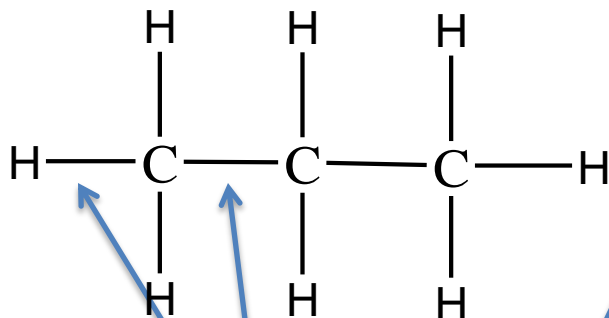
3) Weak interaction among the same compound

4) Insoluble in water

Physical properties of the alkanes

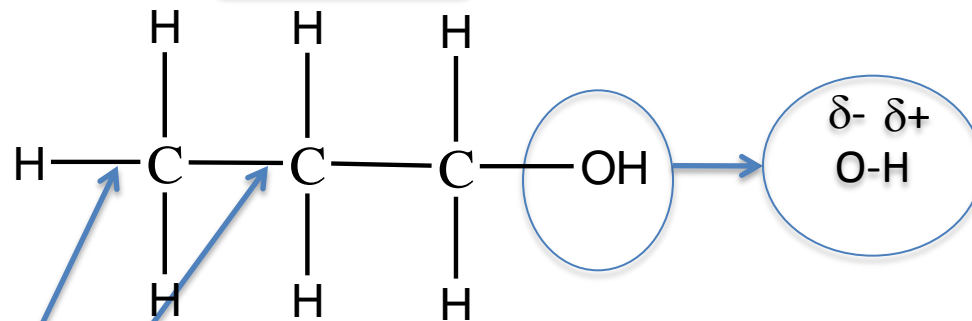
1) Non-polar

alkane

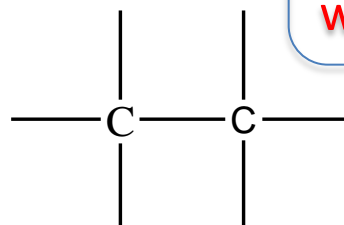


Covalent bonds

alcohol



Different electronegativity
attract the shared electron
with different strength



When two atoms with same
element are joined by a
covalent bond

Electrons are shared equally
between the two atoms

Physical properties of the alkanes

Lack the ability to form hydrogen bonding

Because of non-polar molecules

Hydrogen bond

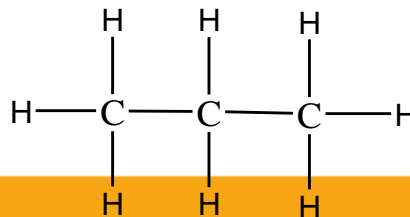
- ❖ dipolar interaction
- ❖ Strong interaction of a hydrogen (H) atom on one molecule to an electronegative atom.
- ❖ Electronegative atoms: N, O or F.

Induced partial positive charge



Attraction between δ^- on X (N, O or F) and δ^+ on H

34



No electronegative atoms

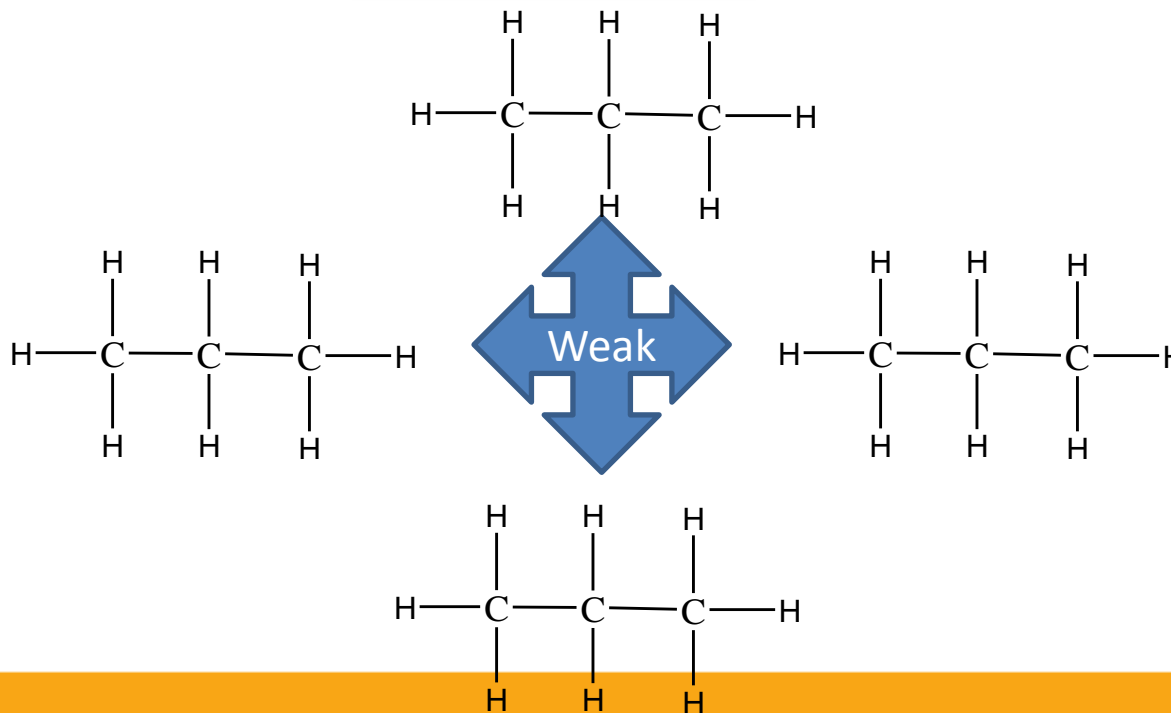
Physical properties of the alkanes

Weak interaction among the same compounds

Non-polar
bonding

Cannot
participate in
dipolar or ionic
interaction

Lack of ability to form
hydrogen bonds



Physical properties of the alkanes

Insoluble in water

Because of non-polar bonding

Lack the ability to form hydrogen bonding



Hexane

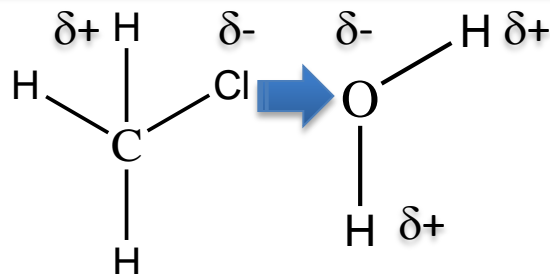
Water

Hydrophobic → water-hating
Lipophilic → oil-loving

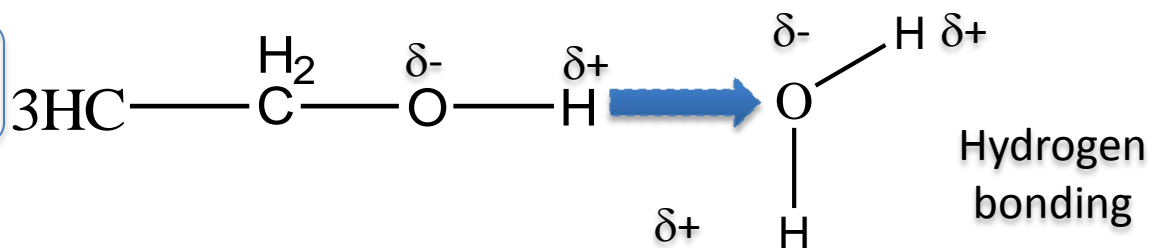
Physical properties of the alkanes

Why non-polar molecules are hydrophobic?

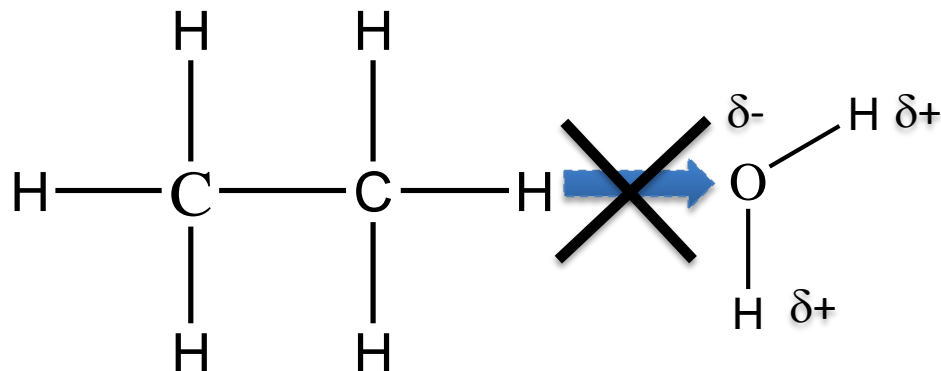
Chloromethane
(polar)



Ethanol (polar)



Ethane (non-polar)



Physical properties of the alkanes

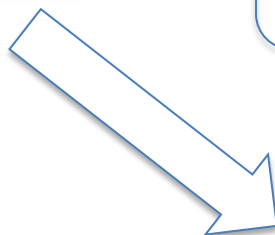
Alkanes are insoluble in water



Alkanes have few direct roles in biological systems



Biological systems are aqueous (water based)



Adding
functional groups

REFERENCES

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- Horton, H.R., Moran, L.A., Scrimgeour, K.G., Perry, M.D. and Rawn J.D. (2006). *Principles of Biochemistry*, 4th Edition. Pearson International Edition.
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MY PROFILE



**Dr Nik Ahmad Nizam Bin Nik Malek,
BSc (Ind. Chem.)(UTM), MSc (Chem)(UTM), PhD (Chem)(UTM), A.M.I.C**

Senior Lecturer,

Department of Biotechnology and Medical Engineering,

Faculty of Biosciences and Medical Engineering,

Universiti Teknologi Malaysia.

Email: niknizam@fbb.utm.my, niknizam@utm.my

Website: <http://www.staff.blog.utm.my/niknizam/>