CHM 102: Introductory Organic Chemistry

General Classification - Organic Compounds



Hydrocarbon

- ✓ Alkane is a hydrocarbon that has only single bonds. Alkanes has a general formula of C_nH_{2n+2} . An alkane in the shape of a ring is called a cycloalkane.
- ✓ Alkene is a compound that has at least one double bond. Alkene general formula is C_nH_{2n} .
- Alkyne is a compound that has at least one triple bond. A straight chain alkyne with one triple bond has the formula C_nH_{2n-2} .



Cycloalkanes



cyclopropane





cyclopentane



cyclohexane



cyclohexane



cyclooctane

Name	Molecular formula	Name	Molecular formula
Methane	CH ₄	Undecane	C ₁₁ H ₂₄
Ethane	C_2H_6	Dodecane	$C_{12}H_{26}$
Propane	C_3H_8	Tridecane	$C_{13}H_{28}$
Butane	C_4H_{10}	Tetradecane	$C_{14}H_{30}$
Pentane	$C_{5}H_{12}$	Pentadecane	$C_{15}H_{32}$
Hexane	$C_{6}H_{14}$	Hexadecane	$C_{16}H_{34}$
Heptane	$C_{7}H_{16}$	Heptadecane	$C_{17}H_{36}$
Octane	$C_{8}H_{18}$	Octadecane	$C_{18}H_{38}$
Nonane	C_9H_{20}	Nonadecane	$C_{19}H_{40}$
Decane	$C_{10}H_{22}$	Eicosane	$C_{20}H_{42}$

Nomenclature of alkane

- ✓ Identify the parent chain (longest carbon chain) and the substituents (groups attached to the parent chain).
- ✓ Identify the 'branches' on the longest carbon chain and name them accordingly.
- ✓ Number the carbon atoms on the longest carbon chain to describe the positions of the branches – use the lowest numbers possible.
- Each substituent is given a name and a number.
 The number shows the carbon atom to which the substituent is attached.

- If the substituent appears more than once, the number of each carbon of the parent chain on which the substituent occur is given. In addition, the number of times in which the substituent occur is given by a prefix di-, tri-, tetra-, penta-, etc.
- ✓ If there are 2 or more substituent, they are listed in alphabetical order. (Ignore prefix like di-, tri-, tetra-, etc, or sec-, tert-, etc, when alphabetizing).



(a) Write the structural formulae of: (i) 2-bromo-3chloro3-methylpentane (ii) 4-ethyl-2-methylheptane
(iii) 2,2,5-trimethyloctane (iv) 2,3,4-trimethylheptane.

(b) Name the following organic compounds



Shapes of alkane molecules



Structural isomerism in alkanes

Two or more compounds that have the same molecular formula but different orders of attachment of atoms are called structural isomer.





2-methylpropane (bp -11.2°C)

Show all the possible isomers of : 1) Pentane (C_5H_{12}) 2) Hexane (C_6H_{14})

Preparation of alkane

1. Wurtz reaction

$$2 R - X - Na \rightarrow R - R$$



Reaction of alkane





Sources of alkanes

- ✓ Alkanes are obtained from crude oil and natural gas.
- ✓ Natural gas contains 60–90% methane.
- ✓ Crude oil is a mixture of many carbon compounds with different chain lengths.
- ✓ The oil is therefore separated into groups of compounds with roughly the same chain length in an oil refinery.
- ✓ The technique that is used to refine the oil is called fractional distillation.

Fractional distillation of crude oil

- The oil is heated and passed into a tall fractionating column.
- Compounds with large molecules and high boiling points are collected at the bottom of the tower, whereas the more volatile components, with smaller molecules, are collected near the top.
- ✓ Each group of compounds collected is called a fraction.
- ✓ Each fraction is still a complicated mixture, since it contains alkanes of a range of carbon numbers and isomers of each carbon number.
- ✓ In addition to alkanes, crude oil contains some cycloalkanes and aromatic compounds the proportion of each present depends upon the source of the oil.

Fractionating column



Alkenes

- ✓ Alkene molecules contain a double bond between carbon atoms.
- ✓ They have the general formula C_nH_{2n} and their names end in 'ene'.
- ✓ The first three (ethene, propene, and butene) are gases at 25°C.



Nomenclature of Alkenes

- ✓ The IUPAC names of alkenes are formed by changing the –an- infix of the parent alkane to –en-. Hence CH₂=CH₂ is named ethene and CH₃CH=CH₂ is named propene.
- ✓ According to the IUPAC system, the longest carbon chain that contains the double bond is numbered to give the carbon atoms of the double bond the lowest possible numbers.
- The location of the double bond is indicated by the number of the first carbon of the double bond. Branched or substituted alkenes are named in the same way as alkanes.
- The carbon atoms are numbered, substituent groups are located and named, the double bond is located, and the parent chain is named.

Exercise Name the following compounds:



(d)





Preparation of Alkene

1. Dehydrogenation of alkylhalides



2. Dehalogenation of vicinal dihalides.







4. Reduction of Alkynes



Reactions of alkene

1. Hydrogenation



2. Halogenation



 $X_2 = Cl_2, Br_2$

3. Addition of hydrogen halide.



HX = HCl, HBr, HI

Markonikoff rule: The hydrogen of the acid attach itself to the carbon which already has the greatest number of hydrogen. In the presence of peroxide, HBr will undergo anti-Markovnikov addition.

4. Addition of sulphuric acid



5. Addition of water



6. Halohydrin formation



X = CI, Br

7. Oxymecuration – Demercuration



8. Hydroboration – Oxidation







9. Hydroxylation



Ozonolysis

- ✓ Ozonolysis or ozonation is the cleavage of an alkene by ozone (O_3).
- \checkmark It is a cycloaddition that destroys bonds
- ✓ ozone is a powerful oxidant and cleaves the alkene to make two carbonyl compounds.
- ✓ Ozone s a 1,3-dipole and does typical 1,3- dipolar cycloadditions with alkenes.

Structure of ozone:



Ozonolysis reactions



Ozonolysis of cyclohexenes is particularly useful as it gives 1,6-dicarbonyl compounds that are otherwise difficult to make.



In the simplest case we get hexane 1,6-dioic acid (adipic acid) a monomer for nylon manufacture.

Alkynes





 $CaC_2 + H_2O \longrightarrow HC \equiv CH + Ca(OH)_2$

Reaction of alkynes

1. Hydrogenation



2. Halogenation



3. Addition of hydrogen halide



4. Addition of water (hydration)



Benzene

Preparation of benzene

1. Ring formation



2. Cyclisation



3. Elimination



Reactions of benzene

1. Nitration



X = Cl, Br

4. Friedel-Crafts Alkylation

$$\langle \bigcirc \rangle$$
 + RCl $\xrightarrow{\text{Fe}}$ $\langle \bigcirc \rangle$ -R + HCl

5. Friedel-Crafts acylation (also hydrogenation)

$$\langle \bigcirc + ROCI \longrightarrow \langle \bigcirc -COR + HCI$$

6. Bromination



7. Combustion

$$2 \bigcirc + (15 - n) O_2 \longrightarrow (12 - n) CO_2 + 6H_2O + nC$$

Alcohols

(or 1-propanol)

General formula CH₃CHCH₃ $C_nH_{2n+1}OH$ or R-OH OH CH₃-CH-OH CH₃CH₂CH₂-OH propan-1-ol ethanol

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propan-2-ol
(or 2-propanol)
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CH₃CH₂CH₂CH₂-OH

1-butanol (or butan-1-ol) CH₃CHCH₂CH₃ OH

butan-2-ol (or 2-butanol)

Preparation of Alcohols

1. Addition of hydroxide

R-OH R-X NaOH ++NaX 2. Grignads reagents \blacktriangleright R-CH₂-O-Mg-X H-CHO + R-Mg-X $R-CH_2-O-Mg-X + HX$ $R-CH_2-OH + MgX_2$ primary alcohol Ŗ' MgX_2 +R-Ç-OH + R'-Mg-XR-CHO Ή secondary alcohol R $R_2C=O + R'-Mg-X$ ► R-C-OH + MgX_2 R' tertiary alcohol

3. Hydration of alkenes



4. Reaction of amines with nitrous acid

R-NH₂ + HO-NO $\xrightarrow{\text{NaNO}_2}_{\text{H+}}$ ROH + N₂ + H₂O 5. Oxymecuration – Demecuration $\downarrow c = c + H_2O \xrightarrow{\text{Hg(OAc)}_2} - \frac{|c|}{|c|} + \frac$

Markovnikov addition

6. Hydroboration – Oxidation



Anti-Markovnikov addition

Reaction of Alcohols

1. Reaction with hydrogen halides

$$R-OH + HX \longrightarrow RX + H_2O$$

Reactivity of HX: HI > HBr > HClReactivity of ROH: allyl, $benzyl > 3^{o} > 2^{o} > 1^{o}$ 2. Reaction with Phosphorous trihalide

4. Ester formation

 $R-OH + R'COX \longrightarrow ROOCR' + HX$

 $R-OH + R'COOH \longrightarrow ROOCR' + H_2O$

5. Reaction with active metals

 $R-OH + M \longrightarrow RO^{-}M^{+} + 1/_2 H_2$

6. Oxidation

