11. Organic Chemistry

Many areas rely on organic chemistry

- biology
- petroleum industry
- polymers
- genetic engineering
- agriculture
- pharmacology
- consumer products
Organic Chemistry

Organic: overused word

Organic can be biological or chemical term

Biology:
anything living or has lived

Chemistry:
most substances containing carbon
Originally the study of chemicals extracted from living systems
Today, organic chemistry is the study of compounds containing carbon

Synthesis of urea from ammonium cyanate

\[ \text{NH}_4\text{OCN} \xrightarrow{\Delta} \text{C} \text{H}_2\text{N}-\text{NH}_2 \]

Wohler, 1928
IMPORTANCE OF CARBON

basis for all life
stable covalent bonds catenation
forms $C\equiv C$  $C\approx C$
forms long chain molecules
$C\equiv C\equiv C\equiv C\equiv C\equiv C\equiv C\equiv C\equiv C\equiv C$
bonds with most elements
infinite number of compounds possible
Rings

cyclohexane
Carbon: the element

Exists in 4 allotropic forms:

1. Amorphous

Soot
2. Graphite

Sheets of rings which can slip over each other.
3. Diamond Tetrahedral arrangement of atoms Hard
4. Spherical Composed of rings
CLASSES OF COMPOUNDS
CLASSES OF COMPOUNDS

Classify by how carbon atoms are arranged & what groups attached

Simplest: hydrocarbons

Divided into 2 classes: aliphatic and aromatic

Methane: $\text{CH}_4$
## ORGANIC COMPOUNDS

Classify by functional group: **specific combinations of atoms**

- **Hydrocarbons**: C & H contain only
- **Alcohols**: $R-OH$
- **Acids**: $R-COOH$
- **Amines**: $R-NH_2$
- **Ketones**: $R(C=O)R$
- **Aldehydes**: $R-CHO$
How do we write formulas, draw structures and name organic compounds?
ORGANIC COMPOUNDS CAN BE COMPLEX

Need a system that shows structure
Must be easy to read

LINE REPRESENTATIONS

Write all atoms in single line
Use subscripts, (), and lines
Show special bonds and branches
Drawing Structures

Molecular formula: \( \text{C}_4\text{H}_{10} \)

Line representation: \( \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \)

Condensed formula

Butane
Drawing Structures

Molecular formula: \( \text{C}_4\text{H}_{10} \)

Line representation: \( \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \)  \( \text{CH}_3(\text{CH}_2)_2\text{CH}_3 \)

Butane
Ball and stick model
Space filling model
Simplest Aliphatic Hydrocarbons

Series of similar C & H compounds

CH\(_4\)  methane
C\(_2\)H\(_6\)  ethane
C\(_3\)H\(_8\)  propane
C\(_4\)H\(_{10}\)  butane
C\(_5\)H\(_{12}\)  pentane
C\(_6\)H\(_{14}\)  hexane

C\(_n\)H\(_{2n+2}\)  Alkanes
# BASE NAMES

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<th>Prefix</th>
<th>No. Carbons</th>
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<td>Meth</td>
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<td>Eth</td>
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<td>Prop</td>
<td>3</td>
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<td>But</td>
<td>4</td>
</tr>
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<td>Pent</td>
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<td>Hex</td>
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<td>Hept</td>
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<tr>
<td>Oct</td>
<td>8</td>
</tr>
<tr>
<td>Non</td>
<td>9</td>
</tr>
<tr>
<td>Dec</td>
<td>10</td>
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Alkanes

Formula and name for 8 carbons?

use standard prefixes and -ane ending

$C_8H_{18}$ octane
<table>
<thead>
<tr>
<th>formula</th>
<th>structure</th>
<th>condensed</th>
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<td>formula</td>
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<td>CH₃CH₂CH₂CH₃</td>
</tr>
</tbody>
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Alkanes
PHYSICAL PROPERTIES

Non-polar molecules
Not water soluble
Low density
Low melting point
Low boiling point
Physical Properties

Non-polar molecules
Not water soluble
Low density
Low melting point
Low boiling point

Increase as the number of C atoms increase
See Table 11.1
SOURCES

Hydrogenation of:
- petroleum
- shale oil
- coal
Methane

Ethane

Propane

Butane
ORGANIC NOMENCLATURE

Naming system must show:

Number of carbons in longest chain
Location of any branches
Where functional groups are (if any)
IUPAC Rules

1. Find longest carbon chain. Use as base name ending - ane

2. Locate any branches on chain. Use base names with yl ending

3. For multiple branches of same type, add di, tri, tetra....
IUPAC RULES

Naming system must show:

4. Show location of each branch with numbers

5. List multiple branches alphabetically
   - the di, tri, tetra don’t count
NAMING ALKANES

Omit hydrogens

H H H H H H H

H-C-C-C-C-C-C-C-C-H

H H H H H H H H H H
NAMING ALKANES

Omit hydrogens

C–C–C–C–C–C–C

1. 6 carbon chain: hex
2. Use -ane ending
3. Name: hexane
NAMING ALKANES

\((\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2\)

Convert from condensed structural formula to simple carbon skeleton.
NAMING ALKANES

$(\text{CH}_3)_2\text{CHCHCH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2$

Convert from condensed structural formula to simple carbon skeleton
NAMING ALKANES

\[(\text{CH}_3)_2\text{CHCHCH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2\]

Convert from condensed structural formula to simple carbon skeleton

1. Two methyl groups - dimethyl
2. 2,5-dimethylhexane
NAMING ALKANES

1. 4 carbon chain: but
2. Use -ane ending
3. Methyl group on second C
4. Name: 2-methylbutane
NAMING ALKANES

\[
\begin{align*}
\text{C-C-C-C-C-C} \\
\quad \quad \quad \quad \quad \quad \downarrow \downarrow \\
\text{C-C} \\
\end{align*}
\]
NAMING ALKANES

C-C-C-C-C-C
     |   |
C-C    3,5-dimethyl heptane
C-C C
NAMING ALKANES

C-C-C-C-C-C
     I    I
C-C    C

3,5-dimethyl heptane

C-C-C-C    C-C-C
     I    I
C-C-C-C-C-C-C-C
     I
C
NAMING ALKANES

3,5-dimethyl heptane

2,3,3,7,8-pentamethyldecan
DRAWING STRUCTURES FROM NAMES

3,5,5-trimethylheptane

Start with base, draw C skeleton

3,5,5-trimethylheptane

C–C–C–C–C–C–C–C

Number carbon atoms
DRAWING STRUCTURES FROM NAMES

3,3,5-trimethylheptane

C₁-C₂-C₃-C₄-C₅-C₆-C₇

Where do the 3 methyl groups go?
DRAWING STRUCTURES FROM NAMES

3,5,5-trimethylheptane

CH$_3$     CH$_3$

C$_1$–C$_2$–C$_3$–C$_4$–C$_5$–C$_6$–C$_7$

CH$_3$
DRAWING STRUCTURES FROM NAMES

3,5,5-trimethylheptane

\[
\begin{align*}
\text{CH}_3 & \quad \text{CH}_3 \\
\text{CH}_3-\text{CH}_2-\text{CH}-\text{CH}_2-\text{C}-\text{CH}_2-\text{CH}_3 \\
\text{CH}_3 \\
\end{align*}
\]

All carbons have 4 bonds
**Structural Isomers**

All have same formula, but different structures and properties

Example

$C_5H_{12}$

C-C-C-C-C

C

This will be more important later where the isomers can result in different functional groups.
Cycloalkanes

Cyclic alkanes

General formula: \( C_nH_{2n} \)

Named as parent alkane with cyclo prefix
REACTIONS OF ALKANES

1. Combustion

\[ \text{CH}_4 + 2 \text{O}_2 \rightarrow \text{CO}_2 + 2 \text{H}_2\text{O} \]

Many alkanes used as fuel

Methane: natural gas
Propane: cooking
Butane: lighters
Gasoline: mixture of hydrocarbons
REATIONS OF ALKANES

2. Halogenation

\[ \text{CH}_4 + \text{Cl}_2 \rightarrow \text{CH}_3\text{Cl} + \text{HCl} \]

Halogen replaces hydrogen

Dichloromethane: paint stripper
Chloroform: anesthesia
1,2-dichloroethane: dry cleaning
Alkyl Halides

Alkanes with at least 1 halogen replacing hydrogen

General formula: $R-X$

A halogen $F, Cl, Br, I$

Any alkane chain

Structure and naming similar to alkanes
# Alkyl Halides

<table>
<thead>
<tr>
<th>Halogen</th>
<th>Name</th>
<th>Symbol</th>
</tr>
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<tbody>
<tr>
<td>fluorine</td>
<td>fluoro</td>
<td>−F</td>
</tr>
<tr>
<td>chlorine</td>
<td>chloro</td>
<td>−Cl</td>
</tr>
<tr>
<td>bromine</td>
<td>bromo</td>
<td>−Br</td>
</tr>
<tr>
<td>iodine</td>
<td>iodo</td>
<td>−I</td>
</tr>
</tbody>
</table>
**ALKYL HALIDES**

Give name and carbon number for halide just like a side branch

- C–C–F
  - 1-fluoroethane
- C–C–C
  - 2-chloropropane
- C–C–C–C–C–C
  - 1-bromo-2-methylpentane
  - C–Br
ALKENES AND ALKYNES

Unsaturated hydrocarbons
Contain C–C multiple bonds

Alkenes: \( R-\overset{\equiv}{C}-C-\overset{\equiv}{R} \) \( C_nH_{2n} \)

Alkynes: \( R-\overset{\equiv}{C}=C-\overset{\equiv}{R} \) \( C_nH_{2n-2} \)

Examples: steroids, unsaturated fats, polymers, prostaglandins
ALKENES AND ALKYNES

Geometry

- Alkanes - tetrahedral
- Alkenes - trigonal planar
- Alkynes - linear
COLORED ALKENES

Molecules with many double bonds can be colored

Molecular Weight: 536.89
Molecular Formula: C₄₀H₅₆

Lycopene
NAMING ALKENES

Indicate position of double bond

1. Longest C chain must contain double bond

2. Number carbons so double bond has lowest number

3. Indicate position of double bond
NAMING ALKENES

4. Change ending to \textbf{-ene}

5. Use same rules for side chains and halides
NAMING ALKENES

C = C–C–C

Four carbons: use base but-
Contains double bond: use -ene
Double bond is between first and second: number as 1

1-butene
NAMING ALKENES

Multiple double bonds

Number each double bond

Use -diene for two
-triene for three, etc

\[ \text{C} = \text{C} - \text{C} = \text{C} \]

1,3-butadiene
NAMING ALKYNES

Similar to alkenes

Use ending -yne

C≡C–C–C

1-butyne
MORE EXAMPLES

\[ \text{CH}_3-\text{CH}_2-\text{CH} = \text{CH}-\text{CH}_3 \]

2-pentene
More Examples

CH₃–CH–CH=CH₂

Cl

3-chloro-1-butene
Cl–CH–CH₂–CH₂–CH₃
\[
\text{CH} = \text{CH} – \text{CH₂–CH₃}
\]
5-chloro-3-octene
GEOMETRIC ISOMERS

When two or more arrangements of atoms are possible

Alkanes: rotation about all bonds
         no geometric isomers

Alkenes: rigid bond
         geometric isomers

Alkynes: rigid bond & linear
         geometric isomers
GEOMETRIC ISOMERS

Two possible arrangements

2-butene

cis
largest groups on same side
cis-2-butene

trans
largest groups on opposite sides
trans-2-butene
CIS/TRANS ASSIGNMENTS

1. Locate alkene bond

2. Draw out structure in full
CIS/TRANS ASSIGNMENTS

cis-2-pentene

\[ \text{CH}_3-\text{CH}_2-\text{CH}=\text{CH}-\text{CH}_3 \]
CIS/TRANS ASSIGNMENTS

trans-2-pentene

CH₃-CH₂-CH=CH-CH₃

C = C

CH₃-CH₂-CH=CH-CH₃

C = C

CH₃-CH₂
GEOMETRIC ISOMERS

cis-2-butene

trans-2-butene
REATIONS OF ALKENES

Can react like alkanes
Also react at double bond
Addition reactions common
double bond breaks
atoms added to carbons

\[ R-\text{C}=\text{C}-R \quad \Rightarrow \quad R-\text{C-}\text{C}-R \]
REATIONS OF ALKENES

Hydrogentation

Addition of $H_2$

Forms alkanes

\[ R-\text{C} = \text{C} - R + H_2 \Rightarrow R-\text{C} - \text{C} - R \]

Requires heat, pressure, catalysts - Pt, Pd, Ni
Reactions of Alkenes

Hydrohalogentation

Addition of HX - HF, HCl, HBr, HI

Forms haloalkanes

\[
R-\text{C}=:\text{C}-R + HX \implies R-\text{C}-\text{C}-R
\]

\[
\text{H} \quad \text{X}
\]
AROMATIC HYDROCARBONS

Best represented by benzene

A six carbon ring
Three alternating double bonds
Electrons in bonds spread out
Exists as resonance structure (average)
AROMATIC HYDROCARBONS

Best represented by benzene

Resonance Forms of Benzene
AROMATIC HYDROCARBONS

Fused rings common

benzene

napththalene
AROMATIC HYDROCARBONS

Name benzene derivatives

benzene  chlorobenzene  methylbenzene

nitro: $\text{NO}_2$  amino: $\text{NH}_2$
AROMATIC HYDROCARBONS

Common names

phenol

aniline

toluene
AROMATIC HYDROCARBONS

Disubstituted rings

1,2-dichlorobenzene
1,3- dichlorobenzene
1,4-dichlorobenzene

dichlorobenzene
AROMATIC HYDROCARBONS

Reactions of benzene

A substitution reaction
Functional groups

specific combinations of atoms

- alcohols: $R\text{-OH}$
- acids: $R\text{-COOH}$
- amines: $R\text{-NH}_2$
- ethers: $R\text{-O}\text{-R'}$
- aldehydes: $R\text{-CHO}$
- ketones: $R\text{(C=O)}\text{R'}$
- esters: $R\text{-COOR'}$
Esters

$\text{–OH of acid replaced by –OR}$

$\text{R- COOR}$

$\text{R- C -O -R}$
Isomerism

Stereoisomers
Two types: geometric isomers
optical isomers

Mirror image molecules
enantiomers
cis-trans isomers
Isomerism

Stereoisomers
Compare left and right hands
Non-superimposable mirror images
Distinguish by D- or L- prefix in name
Not optical isomers
Optical isomers
Isomerism

Optical isomers have chiral center or asymmetric carbon atom

\[ \text{Cl} \quad \text{I} \quad \text{C} \quad \text{F} \quad \text{Br} \]

4 different atoms or groups attached
Stereoisomers

Is the red carbon chiral?

Isomerism