Chapter 15
An Introduction to Organic Chemistry, Biochemistry, and Synthetic Polymers

An Introduction to Chemistry
by Mark Bishop
• **Organic chemistry** is the chemistry of carbon-based compounds.

• There are two reasons why there are millions of organic chemicals.
  – Carbon atoms can form strong bonds to other carbon atoms and still form bonds to atoms of other elements.
  – There are many different ways to arrange the same atoms in carbon-based compounds.
Ways to Describe Organic Compounds

- Lewis structures
- Condensed Formulas
  \[ \text{CH}_3\text{CH(\text{CH}_3)\text{CH}_3} \]
- Line Drawings
Hydrocarbons (compounds composed of carbon and hydrogen) in which all of the carbon-carbon bonds are single bonds.
Pre-ignition Knock and Octane Rating

If the gasoline-air mixture ignites too soon, before the peak of the stroke of the piston, the piston pushes the crankshaft in the opposite direction, causing a vibration or "pre-ignition knock".

If the gasoline-air mixture ignites at (or just past) the peak of the stroke of the piston, the crankshaft is turned, which ultimately turns the wheels.

Straight-chain hydrocarbons are more likely to pre-ignite, so a gasoline that has a high percentage of straight-chain hydrocarbons has a low octane rating.

Branched-chain hydrocarbons are less likely to pre-ignite, so a gasoline that has a high percentage of branched-chain hydrocarbons has a high octane rating.
Steps to Octane Rating

• Measure efficiency and degree of vibration for a test engine running on various percentages of heptane (a straight-chain hydrocarbon) and 2,2,4-trimethylpentane (a branched-chain hydrocarbon).

• Run the same test engine with the gasoline to be tested, and measure its efficiency and degree of vibration.

• Assign an octane rating to the gasoline based on comparison of the efficiency and degree of vibration of the test engine with the gasoline and the various percentages of 2,2,4-trimethylpentane (octane or isooctane) and heptane. For example, if the gasoline runs the test engine as efficiently as 91% 2,2,4-trimethylpentane (octane or isooctane) and 9% heptane, it gets an octane rating of 91.
Hydrocarbons that have one or more carbon-carbon double bonds

The double bond makes this hydrocarbon an alkene.

2-methylpropene (isobutene), \( \text{CH}_2\text{C(CH}_3\text{)}\text{CH}_3 \)
Hydrocarbons that have one or more carbon-carbon triple bonds

The triple bond makes this hydrocarbon an alkyne.

\[ \text{H} - \text{C} \equiv \text{C} - \text{H} \]

Ethylene (acetylene), HCCCH
Benzene
Arenes (or Aromatics) - Compounds that contain the benzene ring

BHT

Benzene rings make these compounds arenes.

TNT
Compounds with one or more -OH groups attached to a hydrocarbon group

Glycerol, HOCH$_2$CH(OH)CH$_2$OH
Carboxylic Acids

Stearic acid, $\text{CH}_3(\text{CH}_2)_{16}\text{CO}_2\text{H}$
Ethers

Two hydrocarbon groups surrounding an oxygen atom

Diethyl ether, $\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\text{CH}_3$
Aldehyde

2-methylbutanal, $\text{CH}_3\text{CH(CH}_3\text{)}\text{CH}_2\text{CHO}$
Ketones

The R’s must be hydrocarbon groups. They cannot be hydrogen atoms.

2-propanone (acetone), $\text{CH}_3\text{COCH}_3$
Esters

The R’ must be a hydrocarbon group. It cannot be a hydrogen atom.

Ethyl butanoate, \( \text{CH}_3\text{CH}_2\text{CH}_2\text{CO}_2\text{CH}_2\text{CH}_3 \)
Amine

Trimethylamine, (CH$_3$)$_3$N
Amides

Ethanamide (acetamide), CH₃CONH₂
Difunctional Compounds - GABA
Types of Biomolecules

• Carbohydrates
  – Monosaccharides (glucose and fructose)
  – Disaccharides (maltose, lactose, and sucrose)
  – Polysaccharides (starch and cellulose)

• Amino Acids and Proteins

• Triglycerides

• Steroids
Monosaccharides

Ketone functional group

\[ \text{Fructose} \]

\[ \text{Glucose} \]

Aldehyde functional group

\[ \text{Galactose} \]

Difference between glucose and galactose

\[ \text{Fructose} \]

\[ \text{Glucose} \]

\[ \text{Galactose} \]
Glucose
Galactose
Fructose
Maltose

Maltose (glucose and glucose)
Sucrose (glucose and fructose)
Lactose (galactose and glucose)
Amylose
Amylopectin or Glycogen
Cellulose
Amino Acids

\[
\begin{align*}
\text{amine group} & : \\
\text{carboxylic acid group} & :
\end{align*}
\]
Alanine
Formation of Ala-Ser-Gly-Cys

Condensation reaction releases water

peptide bonds (amide functional groups)
Protein –
Bovine Pancreatic
Trypsin Inhibitor (BPTI)
Primary and Secondary Protein Structures

• **Primary Structure** = the sequence of amino acids in the protein
• The arrangement of atoms that are close to each other in the polypeptide chain is called the **secondary structure** of protein.
  – Three types
    • $\alpha$-helix
    • $\beta$-sheet
    • irregular
$\alpha$-helix – Secondary Structure

Ball-and-stick model of a portion of the $\alpha$-helical secondary structure of a protein molecule

This ribbon model shows the general arrangement of atoms in a portion of the $\alpha$-helical secondary structure of a protein molecule.

The two models superimposed
β-Sheet Secondary Structure
Tertiary Protein Structure

- The very specific overall shape of the protein called its **tertiary structure**.
- The protein chain is held in its tertiary structure by interactions between the side chains of its amino acids.
  - Disulfide bonds
  - Hydrogen bonds
  - Salt bridges
Disulfide Bonds in Proteins

Position 5

Cys — CH₂ — S

Position 55

S — CH₂ — Cys

Disulfide bond

Cys — CH₂ — S

S — CH₂ — Cys

Helps hold protein in a specific shape
Hydrogen Bonding in Proteins

Hydrogen bond

\[ \text{Ser} \quad \text{CH}_2 \quad \overset{\text{O}}{\text{O}} : \quad \text{H} \quad \overset{\text{O}}{\text{O}} : \quad \text{CH}_2 \quad \text{Ser} \]
Salt Bridge in Proteins

\[ \text{Asp} - \text{CH}_2 - \text{C} - \text{O}^- \quad \text{Salt bridge} \quad + \text{NH}_3 \]

\[ \text{CH}_2 \]
\[ \text{CH}_2 \]
\[ \text{CH}_2 \]
\[ \text{CH}_2 \]

Lys
The Ribbon Structure of the Protein BPTI
Disruption of Salt Bridge

Asp—CH₂—C—O⁻ \quad \text{Salt bridge} \quad \rightarrow \quad \text{Asp—CH₂—C—O⁻}

H⁺ 

\text{CH₂} \\
\text{CH₂} \\
\text{CH₂} \\
\text{Lys} \\

\text{NH₃} 

\quad \rightarrow \\

\quad \text{Asp—CH₂—C—O⁻} \\
\quad \text{H} \\

\quad \text{CH₂} \\
\quad \text{CH₂} \\
\quad \text{CH₂} \\
\quad \text{Lys} \\

\quad \text{NH₃}
Triglycerides (Fats and Oils)

Triglyceride

Hydrocarbon groups
Saturated Triglyceride
- Tristearin
Tristearin – Line Drawing
Unsaturated Triglyceride

Liquid triglycerides are rich in carbon-carbon double bonds.
When there is a double bond between two carbons and when like groups are on different carbons and the same side of the double bond the arrangement is called **cis**.

When the like groups are on opposite sides of the double bond the arrangement is called **trans**.

cis-1,2-difluoroethene  trans-1,2-difluoroethene
Hydrogenation

\[ \text{C} = \text{C} + \text{H}_2 \xrightarrow{\text{Pt}} \text{C} - \text{C} \]
Hydrogenation - Example

Typical vegetable oil molecule - liquid unsaturated triglyceride

\[ + 5H_2(g) \]

Typical molecule in margarine - solid partially hydrogenated triglyceride
Trans Fats

- Hydrogenation is reversible.
- When the double bond is reformed, it is more likely to form the more stable trans form than the less stable cis form.
- Therefore, partial hydrogenated vegetable oils contain trans fats, which are considered to be damaging to your health.

\[
\text{natural cis form} \xrightleftharpoons[H_2/Pt]{} \text{cis form} \xrightleftharpoons[H_2/Pt]{} \text{trans form}
\]
Olestra – a Fat Substitute

olestra

triglyceride
Steroid Skeleton
Cholesterol
Testosterone Formation

Progesterone → 17-Hydroxyprogesterone

Androstenedione → Testosterone
Estradiol

Testosterone → Estradiol
Hydrolysis Reactions

**Ether**

\[
\text{ROCR}' \xrightarrow{\text{H-OH}} \text{ROH} + \text{HOR}'
\]

**Amide**

\[
\text{R}_2\text{NCR}' \xrightarrow{\text{H-OH}} \text{R}_2\text{NH} + \text{HOOCR}'
\]

**Ester**

\[
\text{ROCR}' \xrightarrow{\text{H-OH}} \text{ROH} + \text{HOOCR}'
\]
<table>
<thead>
<tr>
<th>Substance in Food</th>
<th>Products of Digestion</th>
</tr>
</thead>
<tbody>
<tr>
<td>disaccharides</td>
<td>monosaccharides</td>
</tr>
<tr>
<td>polysaccharides</td>
<td>glucose</td>
</tr>
<tr>
<td>protein</td>
<td>amino acids</td>
</tr>
<tr>
<td>Triglycerides (fats and oils)</td>
<td>glycerol and fatty acids</td>
</tr>
</tbody>
</table>
Disruption of Salt Bridge
Amide Hydrolysis

\[
\text{Amide} + \text{Water} \rightleftharpoons \text{Carboxylic acid} + \text{Amine}
\]
Enzymes

- Enzymes are naturally occurring catalysts. **Catalysts** speed chemical changes without being permanently altered themselves.
- The chemicals that they act on are called **substrates**.
- Very specific due to
  - Shape – “Lock and Key”
  - Positions of binding groups, which attract substrates to the active site, the portion of the enzyme where the reaction occurs.
  - Positions of the catalytic groups that speed the reaction.
Enzymes Speed Chemical Reactions

• Provide a different path to products that has more stable intermediates and therefore requires less energy.
• Give the correct orientation every time.
Nylon Formation

\[
\text{Di-amine} + \text{Di-carboxylic acid} \rightarrow \text{Nylon}
\]

\[
\begin{align*}
\text{HO} \quad \text{C} \quad (\text{CH}_2)_x \text{C} \quad \{\text{OH}\} + \quad \text{H} \quad \text{N} \quad (\text{CH}_2)_x \text{N} \quad \text{H} \\
\quad \text{C} \quad (\text{CH}_2)_y \text{C} \quad \{\text{OH}\} + \quad \text{H} \quad \text{N} \quad (\text{CH}_2)_x \text{N} \quad \text{H} \\
\text{repeated many times} \rightarrow \text{Nylon}
\end{align*}
\]

\[n = 40 \text{ to } 110\]

Examples

\[
\begin{align*}
\text{Nylon 66} & \quad \{\text{N} \quad (\text{CH}_2)_6 \text{N} \quad \text{C} \quad (\text{CH}_2)_4 \text{C} \}_n \\
\text{Nylon 610} & \quad \{\text{N} \quad (\text{CH}_2)_6 \text{N} \quad \text{C} \quad (\text{CH}_2)_8 \text{C} \}_n
\end{align*}
\]
Nylon-66

\[
\left(\text{repeated unit}\right)_n
\]

General polymer formula

\[
\left(N\left(\text{CH}_2\right)_6N-C\left(\text{CH}_2\right)_4C\right)_n
\]

Nylon 66
Polyester Formation

\[ \text{Ethylene glycol} + \text{Terephthalic acid} \]
\[ \rightarrow \text{Poly(ethylene terephthalate)} \]
\[ n = \text{a large integer} \]
Polyethylene Formation

\[ n \overset{C=CH}{\longrightarrow} \overset{\text{polymerization}}{\longrightarrow} \overset{\text{R-O-C-C(C-C)C-C-C-C(C-C)C-C-O-R}}{\text{polyethylene}} \]

or more simply

\[ \left( \overset{\text{H}}{\overset{\text{H}}{\overset{\text{C-C}}{\text{H-H}}} \right)_{n} \]

\( n = \text{a very large integer} \)
Poly(vinyl chloride) or PVC

H

\begin{array}{c}
C=\overset{n}{C} \\
H \\
Cl \\
\text{vinyl chloride}
\end{array}

\xrightarrow{\text{polymerization}}

\begin{array}{c}
R-O-C-C(\overset{x}{C-C})_{x}C-C-C-C(\overset{y}{C-C})_{y}C-C-O-R \\
H \quad Cl \quad \overset{x}{H} \quad Cl \quad \overset{y}{H} \quad Cl
\end{array}

\text{or more simply}

\begin{array}{c}
(\overset{n}{C-C})_{n} \\
\overset{n}{H} \quad Cl
\end{array}

n = \text{a very large integer}

\text{poly(vinyl chloride) or PVC}
Addition Polymers

\[ \begin{align*}
\text{Polyethylene} & : (\text{CH}_2\text{CH}_2)_n \\
\text{Polypropylene} & : (\text{CH}_2\text{CH}_2\text{CH}_3)_n \\
\text{Poly(vinyl chloride)} \text{ or PVC} & : (\text{CH}_2\text{CH}_2\text{Cl})_n \\
\text{Polystyrene} & : \text{C}_6\text{H}_5\text{CH}_3
\end{align*} \]
Thermoplastics’ Uses

- Packaging: 32%
- Other: 26%
- Building and construction: 14%
- Consumer products: 13%
- Electrical equipment: 6%
- Transportation equipment: 4%
- Furniture: 5%
Thermosets’ Uses

- Building and construction: 69%
- Transportation: 8%
- Electrical equipment: 4%
- Consumer products: 4%
- Adhesives and coatings: 4%
- Other: 11%
Recycling Codes

1. PET
2. HDPE
3. PVC
4. LDPE
5. PP
6. PS
7. OTHER