ORGANIC CHEMISTRY
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Hydrocarbons are compounds that contain only the elements of carbon and hydrogen.

- **Alkanes** have only C—C single bonds and no functional group.
  - Ethane, CH₃CH₃, is a simple alkane.
- **Alkenes** have a C=C double bond as their functional group.
  - Ethylene, CH₂=CH₂, is a simple alkene.
- **Alkynes** have a C≡C triple bond as their functional group.
  - Acetylene, HC≡CH, is a simple alkyne.
- **Aromatic hydrocarbons** contain a benzene ring, a six-membered ring with three double bonds.
## Hydrocarbons

<table>
<thead>
<tr>
<th>Type of Compound</th>
<th>General Structure</th>
<th>Example</th>
<th>3-D Structure</th>
<th>Functional Group</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alkane</td>
<td>R ─ H</td>
<td>CH₃CH₃</td>
<td><img src="image1.png" alt="3D structure" /></td>
<td></td>
</tr>
<tr>
<td>Alkene</td>
<td>( \text{C} = \text{C} )</td>
<td>( \text{H} ) ─ ( \text{C} = \text{C} ) ─ ( \text{H} )</td>
<td><img src="image2.png" alt="3D structure" /></td>
<td>Carbon-carbon double bond</td>
</tr>
<tr>
<td>Alkyne</td>
<td>─ ( \text{C} = \text{C} ) ─</td>
<td>( \text{H} ) ─ ( \text{C} = \text{C} ) ─ ( \text{H} )</td>
<td><img src="image3.png" alt="3D structure" /></td>
<td>Carbon-carbon triple bond</td>
</tr>
<tr>
<td>Aromatic compound</td>
<td><img src="image4.png" alt="Aromatic structure" /></td>
<td><img src="image5.png" alt="Aromatic structure" /></td>
<td><img src="image6.png" alt="3D structure" /></td>
<td>Benzene ring</td>
</tr>
</tbody>
</table>
Alkanes

Acyclic Alkanes, Cycloalkanes, Nomenclature, Fossil Fuels, Physical Properties, Combustion
Alkanes are hydrocarbons having only C–C and C–H single bonds.

The carbons of an alkane can be joined together to form chains or rings of atoms.

Alkanes are the simplest organic molecules.
Alkanes

- Alkanes that contain chains of carbon atoms but no rings are called **acyclic alkanes**.
  - An **acyclic alkane** has the molecular formula $C_nH_{2n+2}$, where $n$ is the number of carbons it contains.
  - **Acyclic alkanes** are also called saturated hydrocarbons because they have the maximum number of hydrogen atoms per carbon.

- **Cycloalkanes** contain carbons joined in one or more rings.
  - Since a cycloalkane has two fewer H’s than an acyclic alkane with the same number of carbons, its general formula is $C_nH_{2n}$.
Undecane and cyclohexane are examples of two naturally occurring alkanes.

- **Undecane** is an acyclic alkane with molecular formula C\textsubscript{11}H\textsubscript{24} and is a *pheromone*, a chemical substance used for communication in a specific animal species, most commonly an insect population. Secretion of undecane by a cockroach causes other members of the species to aggregate.

- **Cyclohexane**, a cycloalkane with molecular formula C\textsubscript{6}H\textsubscript{12}, is one component of the mango, the most widely consumed fruit in the world.
Acyclic Alkanes Having Fewer Than 5 Carbons

- **Methane**, $\text{CH}_4$, has a single carbon atom surrounded by four hydrogens to give it four bonds.

- **Ethane**, $\text{CH}_3\text{CH}_3$, has two carbon atoms joined together by a single bond. Each carbon is also bonded to three hydrogens to give it four bonds total.

- The shape around atoms in organic molecules is determined by counting groups. Since each carbon in an alkane is surrounded by four atoms, each carbon is **tetrahedral**, and all bond angles are 109.5°.
\[
\begin{align*}
\text{CH}_4 & \quad \text{methane} \quad \begin{array}{c}
\text{H} \\
\text{H} \\
\text{H} \\
\text{H}
\end{array} \\
\begin{array}{c}
\text{H} \\
\text{C} \\
\text{C} \\
\text{H}
\end{array} & \begin{array}{c}
\text{H} \\
\text{H} \\
\text{H}
\end{array} \\
\begin{array}{c}
\text{H} \\
\text{H} \\
\text{H}
\end{array} & \text{3-D representation} \\
\begin{array}{c}
\text{H} \\
\text{H} \\
\text{H}
\end{array} & \text{ball-and-stick model}
\end{align*}
\]

\[
\begin{align*}
\text{CH}_3\text{CH}_3 & \quad \text{ethane} \quad \begin{array}{c}
\text{H} \\
\text{H} \\
\text{H}
\end{array} \\
\begin{array}{c}
\text{H} \\
\text{C} \\
\text{C}
\end{array} & \begin{array}{c}
\text{H} \\
\text{H} \\
\text{H}
\end{array} \\
\begin{array}{c}
\text{H} \\
\text{H} \\
\text{H}
\end{array} & \text{3-D representation} \\
\begin{array}{c}
\text{H} \\
\text{H} \\
\text{H}
\end{array} & \text{ball-and-stick model}
\end{align*}
\]
Acyclic Alkanes Having Fewer Than 5 Carbons

- There are two different ways to arrange four carbons, giving two compounds with molecular formula \( \text{C}_4\text{H}_{10} \).
  - **Butane**, \( \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \), has four carbon atoms in a row. **Butane is a straight-chain alkane**, an alkane that has all of its carbons in one continuous chain.
  - **Isobutane**, \( (\text{CH}_3)_3\text{CH} \), has three carbon atoms in a row and one carbon bonded to the middle carbon. **Isobutane is a branched-chain alkane**, an alkane that contains one or more carbon branches bonded to a carbon chain.
Butane and isobutane are isomers, two different compounds with the same molecular formula.

They belong to one of the two major classes of isomers called constitutional isomers.
Acyclic Alkanes Having 5 or More Carbons

- As the number of carbon atoms in an alkane increases, so does the number of isomers.
- There are three constitutional isomers for the five-carbon alkane, each having molecular formula C₅H₁₂:
  - pentane,
  - isopentane (or 2-methylbutane), and
  - neopentane (or 2,2-dimethylpropane).
CH₃CH₂CH₂CH₂CH₃  pentane

CH₃-C-CH₂CH₃  isopentane
(2-methylbutane)

CH₃-C-CH₃  neopentane
(2,2-dimethylpropane)
With alkanes having five or more carbons, the names of the straight-chain isomers are derived from Greek roots: pentane for five carbons, hexane for six, and so on.

The suffix -ane identifies a molecule as an alkane.

The remainder of the name meth-, eth-, prop-, and so forth indicates the number of carbons in the long chain.
### Straight-Chain Alkanes

<table>
<thead>
<tr>
<th>Number of C’s</th>
<th>Molecular Formula</th>
<th>Structure</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>CH(_4)</td>
<td>CH(_4)</td>
<td>methane</td>
</tr>
<tr>
<td>2</td>
<td>C(_2)H(_6)</td>
<td>CH(_3)CH(_3)</td>
<td>ethane</td>
</tr>
<tr>
<td>3</td>
<td>C(_3)H(_8)</td>
<td>CH(_3)CH(_2)CH(_3)</td>
<td>propane</td>
</tr>
<tr>
<td>4</td>
<td>C(<em>4)H(</em>{10})</td>
<td>CH(_3)CH(_2)CH(_2)CH(_3)</td>
<td>butane</td>
</tr>
<tr>
<td>5</td>
<td>C(<em>5)H(</em>{12})</td>
<td>CH(_3)CH(_2)CH(_2)CH(_2)CH(_3)</td>
<td>pentane</td>
</tr>
<tr>
<td>6</td>
<td>C(<em>6)H(</em>{14})</td>
<td>CH(_3)CH(_2)CH(_2)CH(_2)CH(_2)CH(_3)</td>
<td>hexane</td>
</tr>
<tr>
<td>7</td>
<td>C(<em>7)H(</em>{16})</td>
<td>CH(_3)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_3)</td>
<td>heptane</td>
</tr>
<tr>
<td>8</td>
<td>C(<em>8)H(</em>{18})</td>
<td>CH(_3)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_3)</td>
<td>octane</td>
</tr>
<tr>
<td>9</td>
<td>C(<em>9)H(</em>{20})</td>
<td>CH(_3)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_3)</td>
<td>nonane</td>
</tr>
<tr>
<td>10</td>
<td>C(<em>{10})H(</em>{22})</td>
<td>CH(_3)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_3)</td>
<td>decane</td>
</tr>
</tbody>
</table>
How are organic compounds named? Long ago, the name of a compound was often based on the plant or animal source from which it was obtained.

- For example, the name allicin, the principal component of the odor of garlic, is derived from the botanical name for garlic, *Allium sativum*. With the isolation and preparation of thousands of new organic compounds it became obvious that each organic compound must have an unambiguous name.

A systematic method of naming compounds (a system of nomenclature) was developed by the International Union of Pure and Applied Chemistry. It is referred to as the IUPAC system of nomenclature.
The Basic Features of Alkane Nomenclature

- Although the names of the straight-chain alkanes having 10 carbons or fewer were already given previously, we must also learn how to name alkanes that have carbon branches, called substituents, bonded to a long chain.

- The names of these organic molecules have three parts.
  - The **parent name** indicates the number of carbons in the longest continuous carbon chain in the molecule.
  - The **suffix** indicates what functional group is present.
  - The **prefix** tells us the identity, location, and number of substituents attached to the carbon chain.
The names of the straight-chain alkanes consist of two parts.
- The suffix -ane indicates that the compounds are alkanes.
- The remainder of the name is the parent name, which indicates the number of carbon atoms in the longest carbon chain.
- The parent name for one carbon is meth-, for two carbons is eth-, and so on. Thus, we are already familiar with two parts of the name of an organic compound.
Naming Substituents

- Carbon substituents bonded to a long carbon chain are called alkyl groups.
- An alkyl group is formed by removing one hydrogen from an alkane.
- An alkyl group is a part of a molecule that is now able to bond to another atom or a functional group. To name an alkyl group, change the -ane ending of the parent alkane to -yl. Thus, methane (CH$_4$) becomes methyl (CH$_3$—) and ethane (CH$_3$CH$_3$) becomes ethyl (CH$_3$CH$_2$—).
Naming Substituents

- Removing one hydrogen from an end carbon in any straight-chain alkane forms other alkyl groups named in a similar fashion.

- Thus, propane (CH$_3$CH$_2$CH$_3$) becomes propyl (CH$_3$CH$_2$CH$_2$-), and butane (CH$_3$CH$_2$CH$_2$CH$_3$) becomes butyl (CH$_3$CH$_2$CH$_2$CH$_2$-).
# Some Common Alkyl Groups

<table>
<thead>
<tr>
<th>Number of C’s</th>
<th>Structure</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>CH₃⁻</td>
<td>methyl</td>
</tr>
<tr>
<td>2</td>
<td>CH₃CH₂⁻</td>
<td>ethyl</td>
</tr>
<tr>
<td>3</td>
<td>CH₃CH₂CH₂⁻</td>
<td>propyl</td>
</tr>
<tr>
<td>4</td>
<td>CH₃CH₂CH₂CH₂⁻</td>
<td>butyl</td>
</tr>
<tr>
<td>5</td>
<td>CH₃CH₂CH₂CH₂CH₂⁻</td>
<td>pentyl</td>
</tr>
<tr>
<td>6</td>
<td>CH₃CH₂CH₂CH₂CH₂CH₂⁻</td>
<td>hexyl</td>
</tr>
</tbody>
</table>
Naming Substituents

Carbon atoms in alkanes and other organic compounds are classified by the number of other carbons directly bonded to them.

- A **primary carbon** ($1^\circ$ carbon) is bonded to one other C atom.
- A **secondary carbon** ($2^\circ$ carbon) is bonded to two other C atoms.
- A **tertiary carbon** ($3^\circ$ carbon) is bonded to three other C atoms.
- A **quaternary carbon** ($4^\circ$ carbon) is bonded to four other C atoms.
Naming Substituents

- Hydrogen atoms are classified as primary (1°), secondary (2°), or tertiary (3°) depending on the type of carbon atom to which they are bonded.
  - A **primary hydrogen** (1° H) is on a C bonded to one other C atom.
  - A **secondary hydrogen** (2° H) is on a C bonded to two other C atoms.
  - A **tertiary hydrogen** (3° H) is on a C bonded to three other C atoms.
The prefix "sec" or "s" is used when the functional group is bonded to a secondary carbon. This prefix is only useful for a four-carbon chain. It is not applicable with a shorter chain, and it is often ambiguous when the chain has five or more carbons.

The prefix "tert" or "t" is used when the functional group is bonded to a tertiary carbon.
From butane:

- $1^\circ$ H’s
  - $2^\circ$ H’s
  - $CH_3CH_2CH_2CH_3$
  - remove a $1^\circ$ H
  - $CH_3CH_2CH_2CH_2$ butyl group

- $1^\circ$ H’s
  - $CH_3CCH_2CH_3$
  - remove a $2^\circ$ H
  - $CH_3CCH_2CH_3$ sec-butyl group

From isobutane:

- $1^\circ$ H’s
  - $1^\circ$ H’s
  - $3^\circ$ H
  - $CH_3CCH_3$
  - remove a $1^\circ$ H
  - $CH_3CCH_2$ isobutyl group

- $1^\circ$ H’s
  - $1^\circ$ H’s
  - $3^\circ$ H
  - $CH_3CCH_3$
  - remove a $3^\circ$ H
  - $CH_3CCH_3$ tert-butyl group
Naming an Acyclic Alkane

- Four steps are needed to name an alkane.
  1. Find the parent carbon chain and add the suffix. Find the longest continuous carbon chain. To the name of the parent, add the suffix -ane for an alkane.
  2. Number the atoms in the carbon chain to give the first substituent the lower number.
  3. Name and number the substituents.
  4. Combine substituent names and numbers + parent + suffix.
6 C’s in the longest chain

6 C’s \[\rightarrow\] hexane

6 C’s in the longest chain of each structure
**CORRECT**

Start numbering here.

```
CH₃─CH─CH₂─CH₂─CH₂─CH₃
```

1 2 3 4 5 6

**INCORRECT**

```
CH₃─CH─CH₂─CH₂─CH₂─CH₃
```

6 5 4 3 2 1

First substituent at C2

First substituent at C5
If two or more identical substituents are bonded to the longest chain, use prefixes to indicate how many: di- for two groups, tri- for three groups, tetra- for four groups, and so forth. The following compound has two methyl groups so its name contains the prefix di- before methyl → dimethyl.
Two numbers are needed, one for each methyl group.

Answer: 2-methylhexane

Answer: 2,3-dimethylhexane
Sample Problem

5-ethyl-2,6-dimethyloctane
Naming New Drugs

- Naming organic compounds has become big business for drug companies.

- The IUPAC name of an organic compound can be long and complex. As a result, most drugs have three names:
  
  - **Systematic**: The systematic name follows the accepted rules of nomenclature; this is the IUPAC name.
  
  - **Generic**: The generic name is the official, internationally approved name for the drug.
  
  - **Trade**: The trade name for a drug is assigned by the company that manufactures it. Trade names are often “catchy” and easy to remember.
Systematic name: 2-[4-(2-methylpropyl)phenyl]propanoic acid
Generic name: ibuprofen
Trade name: xxxxxxxx
Cycloalkanes contain carbon atoms arranged in a ring.

Think of a cycloalkane as being formed by removing two H’s from the end carbons of a chain, and then bonding the two carbons together.

Simple cycloalkanes are named by adding the prefix cyclo- to the name of the acyclic alkane having the same number of carbons.
Cycloalkanes

- Cycloalkanes having three to six carbon atoms are shown in the accompanying figure.
- They are drawn using polygons in skeletal representations.
- Each corner of the polygon has a carbon atom with two hydrogen atoms to give it four bonds.
cyclopropane $C_3H_6$

cyclobutane $C_4H_8$

cyclopentane $C_5H_{10}$

cyclohexane $C_6H_{12}$
Cycloalkanes

- Although we draw cycloalkanes as flat polygons, in reality cycloalkanes with more than three carbons are not planar molecules.
  - Cyclohexane, for example, adopts a puckered arrangement called the **chair** form, in which all bond angles are 109.5°.
Naming Cycloalkanes

- Cycloalkanes are named using the rules in acyclic alkanes, but the prefix **cyclo-** immediately precedes the name of the parent.
Name the ring.
The ring has 6 C’s so the molecule is named as a cyclohexane.
Name and number the substituents.
No number is needed to indicate the location of a single substituent.

methylcyclohexane

butylcyclopentane
Naming Cycloalkanes

- For rings with **more than one substituent**, begin numbering at one substituent, and then give the second substituent the lower number.

- With **two different substituents**, number the ring to assign the lower number to the substituents alphabetically.
• Place CH$_3$ groups at C1 and C3.

1,3-dimethylcyclohexane

(not 1,5-dimethylcyclohexane)

Earlier letter $\rightarrow$ lower number

• ethyl group at C1
• methyl group at C3

1-ethyl-3-methylcyclohexane

(not 3-ethyl-1-methylcyclohexane)
1-ethyl-2-propylcyclopentane
Fossil Fuels

- Many alkanes occur in nature, primarily in natural gas and petroleum.
- Both of these fossil fuels serve as energy sources, formed long ago by the degradation of organic material.
- **Natural gas** is composed largely of **methane** (60-80% depending on its source), with lesser amounts of ethane, propane, and butane. These organic compounds burn in the presence of oxygen, releasing energy for cooking and heating.
Fossil Fuels

- **Petroleum** is a complex mixture of compounds, most of which are hydrocarbons containing 1-40 carbon atoms.
- Distilling crude petroleum, a process called **refining**, separates it into usable fractions that differ in boiling point.
- Most products of petroleum refining provide fuel for home heating, automobiles, diesel engines, and airplanes. Each fuel type has a different composition of hydrocarbons.
Fossil Fuels

- **Gasoline:** $C_5H_{12} - C_{12}H_{26}$
  - Primarily as a fuel in internal combustion engines.

- **Kerosene:** $C_{12}H_{26} - C_{16}H_{34}$
  - Also known as paraffin, lamp oil and coal oil.
  - Widely used as a fuel in industry, households, to power jet engines of aircraft (jet fuel) and some rocket engines.

- **Diesel fuel:** $C_{15}H_{32} - C_{18}H_{38}$
  - Liquid fuel used in diesel engines.
Fossil Fuels

- Petroleum provides more than fuel.
  - About 3% of crude oil is used to make plastics and other synthetic compounds, including drugs, fabrics, dyes, and pesticides.
  - These products are responsible for many of the comforts we now take for granted in industrialized countries.
  - Imagine what life would be like without air-conditioning, refrigeration, anesthetics, and pain relievers, all products of the petroleum industry.
a) **An oil refinery.** At an oil refinery, crude petroleum is separated into ractions of similar boiling point.

(b) **A refinery tower.** As crude petroleum is heated, the lower-boiling components come off at the top of the tower, followed by fractions of higher boiling point.
1 gallon = 3.78541 liter

Barrel of crude oil

- petroleum starting materials for chemical synthesis (1.25 gal)
- asphalt and road oil (1.3 gal)
- boiler oil (2.9 gal)
- lubricants, waxes, solvents (4.2 gal)
- jet fuel (4.2 gal)
- diesel and home heating oil (8.4 gal)
- gasoline (19.7 gal)

products made from petroleum
Fossil Fuels

- Energy from petroleum is *nonrenewable*, and the remaining known oil reserves are limited.

- Given our dependence on petroleum, not only for fuel, but also for the many necessities of modern society, it becomes obvious that we must both conserve what we have and find alternate energy sources.
Physical Properties of Alkanes

- Alkanes contain only nonpolar C–C and C–H bonds, so they exhibit only weak intermolecular forces. As a result, alkanes have low melting points and boiling points.

- Low molecular weight alkanes are gases at room temperature, and alkanes used in gasoline are all liquids.

- The melting points and boiling points of alkanes increase as the number of carbons increases.
**Physical Properties of Alkanes**

- Increased surface area increases the force of attraction between molecules, thus raising the boiling point and melting point. This is seen in comparing the boiling points of three straight chain alkanes.

<table>
<thead>
<tr>
<th></th>
<th>CH₃CH₂CH₂CH₃</th>
<th>CH₃CH₂CH₂CH₂CH₃</th>
<th>CH₃CH₂CH₂CH₂CH₂CH₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>Butane</td>
<td>CH₃CH₂CH₂CH₃</td>
<td>CH₃CH₂CH₂CH₂CH₃</td>
<td>CH₃CH₂CH₂CH₂CH₂CH₃</td>
</tr>
<tr>
<td>bp = –0.5 °C</td>
<td>bp = 36 °C</td>
<td>bp = 69 °C</td>
<td></td>
</tr>
</tbody>
</table>

Increasing surface area
Increasing boiling point
Physical Properties of Alkanes

- Because nonpolar alkanes are water insoluble and less dense than water, crude petroleum spilled into the sea from a ruptured oil tanker creates an insoluble oil slick on the surface.

- The insoluble hydrocarbon oil poses a special threat to birds whose feathers are coated with natural nonpolar oils for insulation. Because these oils dissolve in the crude petroleum, birds lose their layer of natural protection and many die.
Combustion

- **Alkanes** are the only family of organic molecules that has no functional group, so alkanes undergo few reactions.

- We consider only one reaction of alkanes.

- Alkanes burn in the presence of oxygen to form carbon dioxide (CO$_2$) and water.

- **Combustion** is an oxidation-reduction reaction.
Combustion

- This is a practical example of oxidation. Every C–H and C–C bond in the starting material is converted to a C–O bond in the product.

\[
2 \text{(CH}_3\text{)}_3\text{CCH}_2\text{CH(CH}_3\text{)}_2 + 25 \text{O}_2 \xrightarrow{\text{flame}} 16 \text{CO}_2 + 18 \text{H}_2\text{O} + \text{energy}
\]

isoctane (high-octane component of gasoline)
Combustion

- Note that the products, $\text{CO}_2 + \text{H}_2\text{O}$, are the same regardless of the identity of the starting material.
  - Combustion of alkanes in the form of natural gas, gasoline, or heating oil releases energy for heating homes, powering vehicles, and cooking food.

- When there is not enough oxygen available to completely burn a hydrocarbon, incomplete combustion may occur and carbon monoxide (CO) is formed instead of carbon dioxide ($\text{CO}_2$).
- **Carbon monoxide** is a poisonous gas that binds to hemoglobin in the blood, thus reducing the amount of oxygen that can be transported through the bloodstream to cells.

\[
2 \text{CH}_4 + 3 \text{O}_2 \xrightarrow{\text{flame}} 2 \text{CO} + 4 \text{H}_2\text{O} + \text{energy}
\]

**Incomplete combustion**
CO can be formed whenever hydrocarbons burn. When an automobile engine burns gasoline, unwanted carbon monoxide can be produced.

Yearly car inspections measure CO and other pollutant levels and are designed to prevent cars from emitting potentially hazardous substances into ambient air.

Carbon monoxide is also formed when cigarettes burn, so heavy smokers have an unhealthy concentration of CO in their bloodstream.
Lipids are biomolecules whose properties resemble those of alkanes and other hydrocarbons.

They are unlike any other class of biomolecules, though, because they are defined by a physical property, not by the presence of a particular functional group.

Lipids are composed of many nonpolar C—H and C—C bonds, and have few polar functional groups.
Lipids have a high energy content, meaning that much energy is released on their metabolism.

Because lipids are composed mainly of C–C and C–H bonds, they are oxidized with the release of energy, just like alkanes are. In fact, lipids are the most efficient biomolecules for the storage of energy.

The combustion of alkanes provides heat for our homes, and the metabolism of lipids provides energy for our bodies.
Alkenes and Alkynes

Nomenclature, Cis-Trans Isomers, Fatty Acids, Oral Contraceptives, Reactions
Alkenes and Alkynes

- Alkenes and alkynes are two families of organic molecules that contain multiple bonds.

- **Alkenes** are compounds that contain a carbon-carbon double bond.
  - The general molecular formula of an alkene is $C_nH_{2n}$, so an alkene has **two** fewer hydrogens than an acyclic alkane.
  - Ethylene ($C_2H_4$) is the simplest alkene.
Since each carbon of ethylene is surrounded by three atoms, each carbon is **trigonal planar**.

All six atoms of ethylene lie in the same plane, and all bond angles are 120°.
**Alkenes and Alkynes**

- **Alkynes** are compounds that contain a carbon-carbon triple bond.

  \[
  \text{Alkyne} \quad \text{H} \text{C} \text{C} \text{C} \text{H} = \quad \text{acylene}
  \]

  - The general molecular formula for an alkyne is \( C_nH_{2n-2} \), so an alkyne has **four** fewer hydrogens than an acyclic alkane.

  \[
  \text{C} \quad \text{C} \quad \text{C} \quad \text{H} \quad \text{H} \quad \text{C} \quad \text{C} \quad \text{H} \quad \text{H} \]

  - Each C is linear.
Alkenes and Alkynes

- Acetylene ($\text{C}_2\text{H}_2$) is the simplest alkyne. Each carbon of acetylene is surrounded by two atoms, making each carbon linear with bond angles of 180°.

- Because alkenes and alkynes are composed of nonpolar carbon-carbon and carbon-hydrogen bonds, their physical properties are similar to other hydrocarbons.

- Like alkanes:
  - Alkenes and alkynes have low melting and boiling points and are insoluble in water.
Alkenes and Alkynes

- Acyclic alkanes are called saturated hydrocarbons, because they contain the maximum number of hydrogen atoms per carbon. In contrast, **alkenes and alkynes are called unsaturated hydrocarbons**.
  - Unsaturated hydrocarbons are compounds that contain fewer than the maximum number of hydrogen atoms per carbon.
  - The multiple bond of an alkene or alkyne is always drawn in a condensed structure.
• Make sure that each carbon of a double bond has three atoms around it, and each carbon of a triple bond has two atoms around it.
Draw a complete structure for each alkene or alkyne.

a. \( \text{CH}_2\equiv\text{CHCH}_2\text{CH}_3 \)
Draw a complete structure for each alkene or alkyne.

b. CH$_3$C≡CCH$_2$CH$_3$

- Draw the triple bond.
- Add a CH$_3$ group.
- Add a CH$_2$CH$_3$ group.
Whenever we encounter a new functional group, we must learn how to use the IUPAC system to name it.

In the IUPAC system:
- An alkene is identified by the suffix -ene.
- An alkyne is identified by the suffix -yne.
Since the compound is an **alkene**, change the -**ane** ending of the parent alkane to -**ene**.

Since the compound is an **alkyne**, change the -**ane** ending of the parent alkane to -**yne**.
Number the carbon chain from the end that gives the multiple bond the lower number.

For each compound, number the chain and name the compound using the first number assigned to the multiple bond.

Numbering the chain from left to right puts the double bond at C1 (not C3).

The alkene is named using the first number assigned to the double bond, making it 1-butene.
Numbering the chain from right to left puts the triple bond at C2 (not C4).

The alkyne is named using the first number assigned to the triple bond, making it 2-hexyne.
Number and name the substituents, and write the name.

3-methyl-1-butene

4-ethyl-2-hexyne
Give the IUPAC name for the following compound.

- Find the longest chain containing both carbon atoms of the multiple bond.

5 C’s in the longest chain \( \rightarrow \) pentene
▪ Number the chain to give the double bond the lower number.
▪ Numbering from right to left is preferred since the double bond begins at C2 (not C3).
▪ The molecule is named as a 2-pentene.
- Name and number the substituents and write the complete name.

- The alkene has two methyl groups located at C2 and C3. Use the prefix di- before methyl → 2,3-dimethyl.

  Answer is 2,3-dimethyl-2-pentene
Cis-Trans Isomers

- Constitutional isomers are possible for alkenes of a given molecular formula.
  
  - For example, there are three constitutional isomers for an alkene of molecular formula \( \text{C}_4\text{H}_8 \); 1-butene, 2-butene, and 2-methylpropene.

\[
\begin{align*}
\text{CH}_2\text{═CHCH}_2\text{CH}_3 & \quad \text{CH}_3\text{CH}═\text{CHCH}_3 & \quad \text{CH}_2═\text{CCH}_3 \\
1\text{-butene} & \quad 2\text{-butene} & \quad 2\text{-methylpropene}
\end{align*}
\]
Cis-Trans Isomers

- 2-Butene illustrates another important aspect about alkenes. There is restricted rotation around the carbon atoms of a double bond.

- With 2-butene, there are two ways to arrange the atoms on the double bond. The two CH₃ groups can be on the same side of the double bond or they can be on opposite sides of the double bond.

- These molecules are different compounds with the same molecular formula; that is, they are isomers.
- When the two CH₃ groups are on the same side of the double bond, the compound is called the **cis isomer**.
- When the two CH₃ groups are on opposite sides of the double bond, the compound is called the **trans isomer**.
- One isomer of 2-butene is called **cis-2-butene**, and the other isomer is called **trans-2-butene**.
Fatty Acids: Saturated and Unsaturated

- Naturally occurring animal fats and vegetable oils are formed from fatty acids. **Fatty acids are carboxylic acids (R-COOH) with long carbon chains of 12-20 carbon atoms.** Because a fatty acid has many nonpolar C—C and C—H bonds and few polar bonds, fatty acids are insoluble in water. There are two types of fatty acids.
  - **Saturated fatty acids** have no double bonds in their long hydrocarbon chains.
  - **Unsaturated fatty acids** have one or more double bonds in their long hydrocarbon chains.
Common Saturated and Unsaturated Fatty Acids

<table>
<thead>
<tr>
<th>Name</th>
<th>Structure</th>
<th>Mp (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stearic acid</td>
<td>CH(_3)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)COOH</td>
<td>71</td>
</tr>
<tr>
<td>(0 C=(\equiv)C)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Oleic acid</td>
<td>CH(_3)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)COOH</td>
<td>16</td>
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<tr>
<td>(1 C=(\equiv)C)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Linoleic acid</td>
<td>CH(_3)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)COOH</td>
<td>-5</td>
</tr>
<tr>
<td>(2 C=(\equiv)C)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Linolenic acid</td>
<td>CH(_3)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)CH(_2)COOH</td>
<td>-11</td>
</tr>
<tr>
<td>(3 C=(\equiv)C)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Fatty Acids: Saturated and Unsaturated

- Generally, double bonds in naturally occurring fatty acids are *cis*.

- The presence of cis double bonds affects the melting point of these fatty acids greatly.
  - As the number of double bonds in the fatty acid *increases*, the melting point *decreases*.
    - The cis double bonds introduce kinks in the long hydrocarbon chain.
    - The larger the number of cis double bonds, the more kinks in the hydrocarbon chain, and the lower the melting point.
Fatty Acids: Saturated and Unsaturated

- Fats and oils are organic molecules synthesized in plant and animal cells from fatty acids. Fats and oils have different physical properties.
  - **Fats** are solids at room temperature. Fats are generally formed from fatty acids having few double bonds.
  - **Oils** are liquids at room temperature. Oils are generally formed from fatty acids having a larger number of double bonds.
Fatty Acids: Saturated and Unsaturated

- Saturated fats are typically obtained from animal sources, while unsaturated oils are common in vegetable sources.
- Thus, butter and lard are formed from saturated fatty acids, while olive oil and safflower oil are formed from unsaturated fatty acids.
- Considerable evidence suggests that an elevated cholesterol level is linked to increased risk of heart disease. Saturated fats stimulate cholesterol synthesis in the liver, resulting in an increase in cholesterol concentration in the blood.
Oral Contraceptives

- The development of synthetic oral contraceptives in the 1960s revolutionized the ability to control fertility.

- Synthetic birth control pills are similar in structure to the female sex hormones estradiol and progesterone, but they also contain a carbon-carbon triple bond.

- Most oral contraceptives contain two synthetic hormones that are more potent than these natural hormones, so they can be administered in lower doses.
ethynylestradiol (a synthetic estrogen)

norethindrone (a synthetic progesterone)

[The carbon-carbon triple bond is drawn in red.]
Alkenes undergo addition reactions. In an addition reaction, new groups X and Y are added to a starting material.

One bond of the double bond is broken and two new single bonds are formed.
Reactions of Alkenes

- **Addition of Hydrogen (Hydrogenation)**
  - Hydrogenation is the addition of hydrogen (H₂) to an alkene.
  - Two bonds are broken—one bond of the carbon-carbon double bond and the H–H bond—and two new C–H bonds are formed.

![Hydrogenation reaction diagram](image)
Reactions of Alkenes

- The addition of $\text{H}_2$ occurs only in the presence of a **metal catalyst** such as palladium (Pd). The metal provides a surface that binds both the alkene and $\text{H}_2$, and this speeds up the rate of reaction.

- Hydrogenation of an alkene forms an **alkane** since the product has only $\text{C}–\text{C}$ single bonds.

**Example**

\[
\text{H}_2\text{C} = \text{C}\text{H} + \text{H}_2 \xrightarrow{\text{Pd}} \text{H}–\text{C}–\text{C}–\text{H}
\]

- ethylene
- ethane

$\text{H}_2$ is added.
Reactions of Alkenes

- Addition of Water (Hydration)
  - Hydration is the addition of water to an alkene.
  - Two bonds are broken—one bond of the carbon–carbon double bond and the H–OH bond and new C–H and C–OH bonds are formed.

\[
\text{alkene} + \text{H–OH} \xrightarrow{\text{H}_2\text{SO}_4} \text{alcohol}
\]

Hydration
Reactions of Alkenes

- Hydration occurs only if a strong acid such as $\text{H}_2\text{SO}_4$ is added to the reaction mixture.
- The product of hydration is an alcohol. For example, hydration of ethylene forms ethanol.

Example: $\text{H}_2\text{C} = \text{C} - \text{H} + \text{H} - \text{OH} \xrightarrow{\text{H}_2\text{SO}_4} \text{H} - \text{C} - \text{C} - \text{H} \rightarrow \text{H} \text{H} \text{H} \text{OH}$

ethylene  ethanol
Reactions of Alkenes

- Ethanol is used as a solvent in many reactions in the laboratory.
- Ethanol is also used as a gasoline additive because, like alkanes, it burns in the presence of oxygen to form CO$_2$ and H$_2$O with the release of a great deal of energy.
- In the addition of H$_2$O to an unsymmetrical alkene, the H atom bonds to the less substituted carbon atom—that is, the carbon that has more H’s to begin with.
Margarine or Butter?

- One addition reaction of alkenes, hydrogenation, is especially important in the food industry.
- It lies at the heart of the debate over which product, butter or margarine, is better for the consumer.
- **Butter** is derived from saturated fatty acids like stearic acid \([\text{CH}_3(\text{CH}_2)_{16}\text{COOH}]\), compounds with long carbon chains that contain only carbon-carbon single bonds. As a result, butter is a solid at room temperature.
Margarine or Butter?

- **Margarine**, on the other hand, is a synthetic product that mimics the taste and texture of butter. It is prepared from vegetable oils derived from unsaturated fatty acids like linoleic acid \([\text{CH}_3(\text{CH}_2)_4\text{CH} \cdot \text{CH} = \text{CH} \cdot \text{CH}_2\text{CH} \cdot \text{CH}(\text{CH}_2)_7\text{COOH}]\).

- **Margarine** is composed mainly of *partially hydrogenated* vegetable oils formed by adding hydrogen to the double bonds in the carbon chain derived from unsaturated fatty acids.
Partial Hydrogenation of the Double Bonds in a Vegetable Oil

Unsaturated vegetable oil
- two C=Cs
- lower melting
- liquid at room temperature

Add H₂ to one C=Cs only.

Partially hydrogenated oil in margarine
- one C=C
- higher melting
- semi-solid at room temperature
Aromatic Compounds
Benzene, Nomenclature, Sunscreens, Phenols as Antioxidants
Aromatic compounds represent another example of unsaturated hydrocarbons.

Aromatic refers to compounds that contain a benzene ring, or rings that react in a similar fashion to benzene.

Benzene, the simplest and most widely known aromatic compound, contains a six-membered ring and three double bonds.
Since each carbon of the ring is also bonded to a hydrogen atom, the molecular formula for benzene is $\text{C}_6\text{H}_6$.

Each carbon is surrounded by three groups, making it trigonal planar. Thus, benzene is a planar molecule, and all bond angles are 120°.
Although benzene is drawn with a six-membered ring and three double bonds, there are two different ways to arrange the double bonds so that they alternate with single bonds around the ring.

Each of these representations is equivalent.

The physical properties of aromatic hydrocarbons are similar to other hydrocarbons. They have low melting and boiling points and are water insoluble.
Nomenclature of Benzene Derivatives

- **Monosubstituted Benzenes**
  - To name a benzene ring with one substituent, name the substituent and add the word *benzene*.
  - Carbon substituents are named as alkyl groups.
  - When a halogen is a substituent, name the halogen by changing the *-ine* ending of the name of the halogen to the suffix *-o*; for example, chlorine → chloro.
Many monosubstituted benzenes, such as those with methyl (CH$_3$), hydroxyl (-OH), and amino (-NH$_2$) groups, have common names that you must learn, too.
Disubstituted Benzenes

- There are three different ways that two groups can be attached to a benzene ring.
- So a prefix —ortho, meta, or para— is used to designate the relative position of the two substituents.
- Ortho, meta, and para are generally abbreviated as o, m, and p, respectively.
1,2-Disubstituted benzene ortho isomer

\[
\text{CH}_2\text{CH}_3 \quad \text{CH}_2\text{CH}_3 \quad \text{CH}_2\text{CH}_3
\]

o-diethylbenzene or 1,2-diethylbenzene

1,3-Disubstituted benzene meta isomer

\[
\text{CH}_2\text{CH}_3 \quad \text{CH}_2\text{CH}_3
\]

m-diethylbenzene or 1,3-diethylbenzene

1,4-Disubstituted benzene para isomer

\[
\text{CH}_2\text{CH}_3 \quad \text{CH}_2\text{CH}_3 \quad \text{CH}_2\text{CH}_3
\]

p-diethylbenzene or 1,4-diethylbenzene
Nomenclature of Benzene Derivatives

- If the two groups on the benzene ring are different, alphabetize the name of the substituents preceding the word benzene.
- If one of the substituents is part of a common root, name the molecule as a derivative of that monosubstituted benzene.

![Chemical structures](image)
Nomenclature of Benzene Derivatives

- **Polysubstituted Benzenes**

  - For three or more substituents on a benzene ring:
    1. Number to give the lowest possible numbers around the ring.
    2. Alphabetize the substituent names.
    3. When substituents are part of common roots, name the molecule as a derivative of that mono-substituted benzene. The substituent that comprises the common root is located at C1, but the “1” is omitted from the name.
Examples of naming polychlorinated benzenes

- Assign the lowest set of numbers.
- Alphabetize the names of all the substituents.

4-chloro-1-ethyl-2-propylbenzene

- Name the molecule as a derivative of the common root aniline.
- Designate the position of the NH₂ group as “1,” and then assign the lowest possible set of numbers to the other substituents.

2,5-dichloroaniline
Sunscreens

- All commercially available sunscreens contain a benzene ring. A sunscreen absorbs ultraviolet radiation and thus shields the skin for a time from its harmful effects.

- Two sunscreens that have been used for this purpose are p-aminobenzoic acid (PABA) and Padimate O.
Phenols as Antioxidants

- A wide variety of phenols, compounds that contain a hydroxyl group bonded to a benzene ring, occur in nature.
- **Vanillin** from the vanilla bean is a phenol, as is **curcumin**, a yellow pigment isolated from turmeric, a tropical perennial in the ginger family and a principal ingredient in curry powder.
- Curcumin has long been used as an anti-inflammatory agent in traditional eastern medicine.
Many phenols are antioxidants, compounds that prevent unwanted oxidation reactions from occurring. Two examples are naturally occurring vitamin E and synthetic BHT (butylated hydroxy toluene).

The OH group on the benzene ring is the key functional group that prevents oxidation reactions from taking place.
Phenols as Antioxidants

- **Vitamin E** is a natural antioxidant found in fish oil, peanut oil, wheat germ, and leafy greens.
  - Although the molecular details of its function remain obscure, it is thought that vitamin E prevents the unwanted oxidation of unsaturated fatty acid residues in cell membranes. In this way, vitamin E helps retard the aging process.

- Synthetic antioxidants such as **BHT (butylated hydroxy toluene)** are added to packaged and prepared foods to prevent oxidation and spoilage. BHT is a common additive in breakfast cereals.
vitamin E

BHT (butylated hydroxy toluene)
A Question

What compounds are obtained by water addition (hydration) to the alkenes?

a. Ethers
b. Alcohols
c. Esters
d. Alkanes
e. Aldehydes

Answer: b
Reference Books