Objectives

- Recognize common elements of organic compounds
- Understand periodic trends in bond formation.
- Assign polarities to molecules based on electronegativity differences.
- Assign 3-D structures to molecules based on bonding of central atom.
- Understand the symbolism of structural formulas and condensed structural formulas for organic molecules.
- Draw expanded, condensed, and line structure formulas for organic compounds.
- Recognize constitutional isomers.

Suggested Problems Ch 11: 1-16, 45-49

Organic Chemistry

- What is organic chemistry?
- What do you think makes it different from inorganic chemistry?
Organic Chemistry

- Why is organic chemistry a separate discipline within chemistry?
- **historical**: scientists at one time believed that a “vital force” present in living organisms was necessary to produce an organic compound
- Then, are organic compounds only found in living organisms? (NO!)

Organic Chemistry

- **Organic chemistry**: the study of the compounds of carbon
  - organic compounds are made up of carbon and only a few other elements
  - chief among these are hydrogen, oxygen, and nitrogen
  - also present are sulfur, phosphorus, and halogens (fluorine, chlorine, bromine, or iodine)

Elements of Organic Chemistry
The sheer number of organic compounds
- Chemists have discovered or made over 10 million organic compounds and an estimated 100,000 new ones are discovered or made each year
- By comparison, chemists have discovered or made an estimated 1.7 million inorganic compounds
- Thus, approximately 85% of all known compounds are organic

What then is different from inorganic chemistry?
- What elements are involved?
  - Salt vs. sugar
  - Chemical formulas:

<table>
<thead>
<tr>
<th>Organic Compounds</th>
<th>Inorganic Compounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bonding is almost entirely covalent</td>
<td>Most have ionic bonds</td>
</tr>
<tr>
<td>May be gases, liquids, or solids with low melting points (less than 360°C)</td>
<td>Most are solids with high melting points</td>
</tr>
<tr>
<td>Most are insoluble in water</td>
<td>Many are soluble in water</td>
</tr>
<tr>
<td>Most are soluble in organic solvents such as diethyl ether, toluene, and dichloromethane</td>
<td>Almost all are insoluble in organic solvents</td>
</tr>
<tr>
<td>Aqueous solutions do not conduct electricity</td>
<td>Aqueous solutions conduct electricity</td>
</tr>
<tr>
<td>Almost all burn</td>
<td>Very few burn</td>
</tr>
<tr>
<td>Reactions are usually slow</td>
<td>Reactions are often very fast</td>
</tr>
</tbody>
</table>
A Look at carbon

- Forms four bonds
  - What is carbon’s electron configuration?
    - 1s²2s²2p²
  - How many valence electrons?
  - How many does it need to be “happy”?
  - How does it get more electrons?
  - Covalent – what does this mean?

Carbon : Bonding

- Bonds arrange as far apart as possible.
  - Why?
    - If molecules with 4 single bonds were flat, what would be the bond angles?
    - Tetrahedron – 109.5°
- What about double or triple bonds?
  - 1 double + 2 single = 4 bonds
  - 2 double bonds = 4 bonds
  - 1 triple + 1 single = 4 bonds
- How many electrons are involved in all the bonds?

Bonding of other elements of organic compounds

- Hydrogen
  - # valence electrons
  - # additional electrons needed:
  - # bonds:
- Nitrogen
  - # valence electrons:
  - # additional electrons needed:
  - # bonds:
- Oxygen
  - # valence electrons:
  - # additional electrons needed:
  - # bonds:
- Halogens
Draw some Lewis structures

- Methane
  - CH₄
- Ammonia
  - NH₃
- Methyl alcohol
  - CH₃OH
- Carbon tetrachloride
  - CCl₄

Carbon Problems

- Insert the correct number of hydrogens to complete the structures.
  a. C−C−C
  b. C−O−C
  c. C=C−C−N

Find the errors

H−C−C−H

H_C_H_C

H_H_H_H

H3C_C_H3

H3C_C_H3

H_H_H

H3C_C_H3

H_H_H
Formulas

- **Molecular**
  - Tell numbers of each atom
    - CH₃
    - C₂H₆

- **Structural**
  - Shows how atoms bonded
    - Expanded
    - Condensed
    - CH₃CH₂

- **Line Structures**
  - Show skeletons of the C-C bonds

Formulas: Example 1

- Write the molecular formula and the condensed structural formula for the following expanded structural formula

```
H H H H
C C C
H H H
```

- Write its condensed structural formula?
  - Find the longest chain of carbon
  - List each C in the chain
  - After each C list all groups attached to it except the next carbon
  - Use parentheses if an attached group contains carbon
  - If the same unit is repeated several times, the condensed formula will sometimes put in in parentheses with a subscript.

Formulas: Example 2

- Write the molecular formula and the condensed structural formula for the following expanded structural formula

```
H H H
H
```

- The condensed formula may still have the branch points drawn out.
A good reason for condensed formulas!

Structural Isomers

- Constitutional isomers
- Compounds with the same molecular formula but different structural formulas.
- Isomers have the same atoms but they are bonded in different orders.
- Bonds must be broken to change between isomers.
- Isomers have different names.
- Isomers have different physical and chemical properties.

Structural Isomers: Examples

What is the difference between these molecules?

- Ethyl Alcohol
  - Molecular formula
  - Molecular weight
  - M.p.: -117 °C
  - B.p.: 78 °C

- Diethyl ether
  - Molecular formula
  - Molecular weight
  - M.p.: -138 °C
  - B.p.: -25 °C

Write the condensed molecular formula for each isomer. (next slide)
Structural Isomers

It doesn’t matter how the bonds are drawn on the page for single bonds. (up or down)

- These are all butane:
- Are they constitutional isomers?
- No! They are the same compound!

\[
\begin{align*}
\text{OH}_3 & \quad \text{CH}_3 & \quad \text{CH}_3 \\
\text{CH}_3 & \quad \text{CH}_3 & \quad \text{CH}_3
\end{align*}
\]

What about?

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

Are these isomers or the same compound?
What is the molecular formula for butane?
Draw the condensed formula for each of the above isomers of butane.
Practice

- Draw the expanded structural formula for $\text{CH}_3(\text{CH}_2)_3\text{CH}_3$

- Draw the expanded structural formula for $\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$

Practice

- Draw the expanded structural formula for $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$
  Write the molecular formula for the above compound.

- Draw the expanded structural formula for $\text{CH}_3\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_3$
  Write the molecular formula for the above compound

Line Structures

- Line structures or line-bond formulas abbreviate C-C bonds as lines.
- Ends of lines and corners represent carbon atoms attached to the appropriate number of hydrogen atoms to give 4 bonds to carbon.
- Write in the carbons represented in each line structure below. Add the appropriate number of hydrogens to each.
Determine the molecular Formula

Go back and draw line structures for the expanded formulas we determined earlier.

Alkanes

Hydrocarbons
Alkane Nomenclature
Alkane properties

Objectives

- Distinguish saturated and unsaturated hydrocarbons.
- Name alkanes, cycloalkanes, and haloalkanes using the IUPAC system.
- Draw structures of hydrocarbons given the IUPAC name.
- Identify 1°, 2°, 3° carbons
- Understand rotation around C-C bonds and how different conformations are possible.
- Understand the cause of cis-trans isomerism in cycloalkanes and distinguish the two isomers.
- Recognize and predict trends in alkane physical properties.

Suggested Problems Ch 11: 17 32a, c, 29 54 59 50
**Hydrocarbons**

- **Hydrocarbon**: a compound composed of only carbon and hydrogen

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**Hydrocarbons**

- Compounds that contain only carbon and hydrogen atoms
  - Methane, propane, octane, ethylene, limonene
- **Saturated**
  - Contain all single bonds
  - Have maximum number of hydrogens
  - Alkanes
- **Unsaturated**
  - Contain double or triple bonds
  - Alkenes, alkynes, arenes (aromatics)

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**Hydrocarbons: Nonpolar**

- Nonpolar molecules
  - Carbon is slightly more electronegative than hydrogen
  - Because the chains contain all carbon surrounded by hydrogen, hydrocarbon molecules are relatively nonpolar.
Alkanes

- Hydrocarbons containing only carbon-carbon single bonds
- General formula
  \[ C_{n}H_{2n+2} \]

- What is the molecular formula for an alkane with three carbons?

<table>
<thead>
<tr>
<th>Number of Carbon Atoms</th>
<th>Prefix</th>
<th>IUPAC Name</th>
<th>Molecular Formula</th>
<th>Condensed Structural Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Meth</td>
<td>Methane</td>
<td>( CH_{4} )</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Eth</td>
<td>Ethane</td>
<td>( C_{2}H_{6} )</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Prop</td>
<td>Propane</td>
<td>( C_{3}H_{8} )</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>But</td>
<td>Butane</td>
<td>( C_{4}H_{10} )</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>Pent</td>
<td>Pentane</td>
<td>( C_{5}H_{12} )</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>Hex</td>
<td>Hexane</td>
<td>( C_{6}H_{14} )</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>Hept</td>
<td>Heptane</td>
<td>( C_{7}H_{16} )</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>Oct</td>
<td>Octane</td>
<td>( C_{8}H_{18} )</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>Non</td>
<td>Nonane</td>
<td>( C_{9}H_{20} )</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>Dec</td>
<td>Decane</td>
<td>( C_{10}H_{22} )</td>
<td></td>
</tr>
</tbody>
</table>

Form an infinite number of straight-chain alkanes by adding C to the end of the chain.
Nomenclature for Straight Chains

- The suffix –ane refers to saturated hydrocarbons.
- Choose the appropriate prefix based on the number of carbons.

<table>
<thead>
<tr>
<th>Prefix</th>
<th>Number of Carbon Atoms</th>
</tr>
</thead>
<tbody>
<tr>
<td>meth-</td>
<td>1</td>
</tr>
<tr>
<td>eth-</td>
<td>2</td>
</tr>
<tr>
<td>prop-</td>
<td>3</td>
</tr>
<tr>
<td>but-</td>
<td>4</td>
</tr>
<tr>
<td>pent-</td>
<td>5</td>
</tr>
<tr>
<td>hex-</td>
<td>6</td>
</tr>
<tr>
<td>hept-</td>
<td>7</td>
</tr>
<tr>
<td>oct-</td>
<td>8</td>
</tr>
<tr>
<td>non-</td>
<td>9</td>
</tr>
<tr>
<td>dec-</td>
<td>10</td>
</tr>
</tbody>
</table>

- To differentiate them from branched chains, straight chains are sometimes given an additional prefix, n- for “normal”.

Straight chain alkanes

- Molecules may have different conformations due to rotation around single bonds.
- Look at butane.

- Least crowded conformation
- Intermediate crowding
- Most crowded conformation

- Remember this rotation does not affect the identity of the compound!

Conformation vs. Configuration

- We have talked about configurational isomers
  - The atoms are bonded differently
  - Bonds must be broken to change from isomer to isomer
- Conformational changes occur by rotating bonds
  - Atoms are bonded the same
  - No bonds are broken
  - Compounds don’t change identity!
Branched Alkanes

- If we do break the bonds in butane and attach the carbons differently we get a branched alkane rather than a straight chain alkane.

\[ \text{\text{CH}_3\text{CH}_2\text{CH}_3} \quad \text{CH}_3\text{CH-C}_3\text{H}_2\text{CH}_3 \]

- These compounds have the same molecular formula but different structures so they are classified as.
- The pieces that branch are named substituents.

Classifying Carbon Atoms

- Looking at the isomers of butane, we can classify each carbon atom according to how many other carbons are bonded to it.

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

- Primary carbons 1 Carbon
- Secondary carbons 2 carbons
- Tertiary carbons 3 carbons

Classify each of the indicated atoms
Nomenclature of Branched Alkanes: Substituents

- **Alkyl group**: a substituent group derived from an alkane by removal of a hydrogen atom
  - commonly represented by the symbol R-
  - named by dropping the -ane from the name of the parent alkane and adding the suffix -yl
  - The dash in the substituent formula shows where the carbon attaches to the parent chain

  **Example**: 
  - `-CH\textsubscript{3}` derived from methane, so named methyl

---

<table>
<thead>
<tr>
<th>Name</th>
<th>Condensed Structural Formula</th>
<th>Name</th>
<th>Condensed Structural Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>methyl</td>
<td><code>-CH\textsubscript{3}</code></td>
<td>isobutyl</td>
<td><code>-CH\textsubscript{2}CHOH\textsubscript{2}CH\textsubscript{3}</code></td>
</tr>
<tr>
<td>ethyl</td>
<td><code>-CH\textsubscript{2}CH\textsubscript{3}</code></td>
<td>sec-butyl</td>
<td><code>-CH\textsubscript{2}HCHOH\textsubscript{2}CH\textsubscript{3}</code></td>
</tr>
<tr>
<td>propyl</td>
<td><code>-CH\textsubscript{2}CH\textsubscript{2}CH\textsubscript{3}</code></td>
<td>tert-butyl</td>
<td><code>-CH\textsubscript{3}HCHOH\textsubscript{2}CH\textsubscript{3}</code></td>
</tr>
<tr>
<td>isopropyl</td>
<td><code>-CH\textsubscript{2}CH\textsubscript{2}CH\textsubscript{2}CH\textsubscript{3}</code></td>
<td></td>
<td></td>
</tr>
<tr>
<td>butyl</td>
<td><code>-CH\textsubscript{2}CH\textsubscript{2}CH\textsubscript{2}CH\textsubscript{2}CH\textsubscript{3}</code></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Substituent Names**

- Look at the propyl group
  - There are two different places to attach the substituent to a parent chain.

- Look at the butyl group
  - How many different carbons on a butyl group can attach to a parent chain?
Nomenclature Rules for Branched Chains

1. Find the longest continuous chain of atoms and name it as the main chain.
   - Make sure you find the longest chain; it may not be drawn in a straight line!
   - If there is more than one chain present with the same number of carbons, use the one with the most branch points as the parent.

2. Number the carbons in the main chain starting from the end nearest a branch (substituent).
   - Make sure each substituent gets the lowest number possible.

3. Give the location and name of each substituent.
   - If there are identical substituents, name them together with the prefix, di-, tri-, tetra, etc.
   - Separate numbers with commas
   - Separate numbers and letters with dashes
Multiple Substituents

4. List the substituents in alphabetical order in front of the parent name.
   - Include the location number of the substituent. Insert dashes between names and numbers except for the last one which becomes one word with the parent name.
   - Alphabetize by the parent name of the alkyl substituent except for isopropyl which you alphabetize by "i".

Naming Alkanes:

Finish naming the compound below.

Naming Alkanes: Practice

Give IUPAC names for the following alkanes

H₂C—CH₂—CH₂—CH₃
Naming Alkanes: Practice

CH₃
CH₂CH₂CH₃
CH₃
CH₃CHCHCH₃
CH₃

More Complicated Example

H₃C CH CH₂CH₂CHCH₃
CH₃ CH₂CH₃
CH₃
CH₃

1. Longest chain is 8, so parent name is octane
2. Number from left to right, not right to left for lowest location numbers
3. Two methyl groups at 2 and 7, 2,7-dimethyl
   One ethyl group at 4, e comes before m
4. 4-ethyl-2,7-dimethyloctane

Problem

• Give the IUPAC name for the molecule shown below

CH₃
H₃C CH CH₂CH₂CHCH₃
CH₃ CH₂CH₃
CH₃
CH₃

Solution

• Longest continuous chain is 7, parent name is heptane
• Side chains are methyl and ethyl
• Lowest location numbers are 3-methyl and 4-ethyl
• Final name is 4-ethyl-3-methylheptane
Hydrocarbon Properties

- Remember, hydrocarbons are nonpolar!
- What kind of forces occur between molecules?

Strength of intermolecular forces
(forces between molecules) increase down the page

- Dispersion forces: nonpolar molecules (hydrocarbons)
- Dipole – dipole: polar molecules (carbonyls)
- Hydrogen bonds: contain H–O,N,F (alcohols) 10X

The forces below are actual bonds between atoms
- Ionic bonds: NaCl 50-100X
- Covalent bonds: >200X

This info is for your extra information. I don’t expect you to know the specific information. Just know that the forces between alkanes are less than b/w polar molecules which are less than those between molecules that H-bond. All of these forces are less than the force between bonded atoms.

Properties of Alkanes:
Boiling and Melting point

- Alkanes have only small forces attracting them to one another so boiling and melting points are low.
  - The small forces between molecules increases as the size of the molecule increases.
  - Longer alkanes - greater boiling and melting points.
### Boiling Point Increase

<table>
<thead>
<tr>
<th>Name</th>
<th>Condensed Structural Formula</th>
<th>M.p. or M.p. (°C)</th>
<th>b.p. (°C)</th>
<th>Density of Liquid at 0°C (g/mL)</th>
</tr>
</thead>
<tbody>
<tr>
<td>methane</td>
<td>CH₄</td>
<td>-182</td>
<td>-184</td>
<td>(g gas)</td>
</tr>
<tr>
<td>ethane</td>
<td>CH₃CH₃</td>
<td>30.1</td>
<td>-83</td>
<td>-68 (g gas)</td>
</tr>
<tr>
<td>propane</td>
<td>CH₃CH₂CH₃</td>
<td>44.1</td>
<td>-49</td>
<td>-42 (g gas)</td>
</tr>
<tr>
<td>butane</td>
<td>CH₃(CH₂)₂CH₃</td>
<td>58.1</td>
<td>-138</td>
<td>0 (g gas)</td>
</tr>
<tr>
<td>pentane</td>
<td>CH₃(CH₂)₃CH₃</td>
<td>72.2</td>
<td>-130</td>
<td>56.626</td>
</tr>
<tr>
<td>hexane</td>
<td>CH₃(CH₂)₄CH₃</td>
<td>86.2</td>
<td>-95</td>
<td>69.069</td>
</tr>
<tr>
<td>heptane</td>
<td>CH₃(CH₂)₅CH₃</td>
<td>100.2</td>
<td>-90</td>
<td>98.0684</td>
</tr>
<tr>
<td>octane</td>
<td>CH₃(CH₂)₆CH₃</td>
<td>114.2</td>
<td>-87</td>
<td>126.703</td>
</tr>
<tr>
<td>nonane</td>
<td>CH₃(CH₂)₇CH₃</td>
<td>128.3</td>
<td>-51</td>
<td>151.718</td>
</tr>
<tr>
<td>decane</td>
<td>CH₃(CH₂)₈CH₃</td>
<td>142.3</td>
<td>-30</td>
<td>174.730</td>
</tr>
</tbody>
</table>

*For comparison, the density of H₂O is 1 g/mL at 4°C.*

### Branched Alkanes

- As branching increases, the molecule becomes more compact.
  - There is less contact between molecules.
  - BP and MP decrease compared to the straight chain alkane with the same number of carbons.

<table>
<thead>
<tr>
<th>Name</th>
<th>bp (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>hexane</td>
<td>68.7</td>
</tr>
<tr>
<td>2-methylpentane</td>
<td>63.3</td>
</tr>
<tr>
<td>3-methylpentane</td>
<td>69.3</td>
</tr>
<tr>
<td>2,3-dimethylbutane</td>
<td>88.0</td>
</tr>
<tr>
<td>2,2-dimethylbutane</td>
<td>89.7</td>
</tr>
</tbody>
</table>

### Properties of Alkanes

#### Solubility and Density

- **Solubility:** A case of “like dissolves like”
  - Alkanes are not soluble in water.
  - Alkanes are soluble in each other.
  - Alkanes are also soluble in other nonpolar organic compounds, such as toluene and diethyl ether.

- **Density:**
  - All liquid and solid alkanes are less dense than water (1.0 g/mL) and, because they are insoluble in water, they float on water.

Have you ever looked at a water puddle at a gas station? What do you see?
Sources of Alkanes

- Natural Gas
- smaller alkanes
- Petroleum – crude oil
- mixture of thousands of compounds
- Fractional distillation – separation of hydrocarbons based on differing boiling points
- Crude oil is heated
  - As the boiling point of a particular alkane is reached, it "boils off" and is removed
- Which alkanes boil at the lowest temperatures?

Source of Alkanes: Petroleum Distillation

Cycloalkanes

- Carbon chains that are connected at the ends form rings or cyclic structures.
- The chain has two fewer hydrogens than straight chain alkanes
  - Formula : C₅H₁₀
- The simplest cycloalkane has three carbons.
  - What is its molecular formula?
  - What would it be named?
  - Cyclo- ?

\[
\begin{align*}
\text{H}_2\text{C} & \\
\text{CH}_2 & \text{CH}_2
\end{align*}
\]
Nomenclature: Substituents

- For one substituent, place the name of substituent at beginning of parent name
  - Methylcyclopentane

Nomenclature

- Multiple substituents
  - Number so all substituents get the lowest number possible.
  - Example:
    - 1,3,4-trimethylcyclopentane or 1,2,4-trimethylcyclopentane?
  - If all substituents could get the same number, number them alphabetically
  - Name example:
Cis-trans isomers

- The bonds in straight chain alkanes can rotate
  - Substituents can point up or down
  - Does rotation change the identity of the compound?
- Can bonds in cyclic compounds rotate?

Cis-Trans isomers

- Rings are "two sided"
- Substituent stays on one side (face) of the ring.
  - On each carbon, one substituent points up and the other down
  - Fill in the rest of the hydrogens

Cis-Trans isomers

- Substituents on different carbons will have one orientation in relation to one another
  - They can be on opposite sides of the ring – trans
  - They can be on the same side of the ring – cis
  - They cannot change from trans to cis without breaking bonds!
  - Changing from trans to cis changes the identity of the compound
Cis-Trans Isomer

- Cis-trans isomers differ in the orientation of atoms in space.
- Cis-trans isomers represent different compounds.
- Bonds must be broken to change from one isomer to the other.
- Which isomer is shown?
- Name this compound.

Nomenclature

- To determine cis or trans, look at substituents attached to ring.
  - The ring must be drawn in perspective.
  - Remember, hydrogen is not considered a substituent.
  - The substituents may not be identical.
- What are the substituent groups in the compound shown?
- Are they cis or trans?
- Insert the hydrogens not shown into the structure.

Properties of Cycloalkanes

Melting and Boiling point

- Cycloalkanes are more rigid than straight chain alkanes.
  - Why do you think this is true?
- Higher boiling points than straight chain alkanes with the same number of carbons.
  - The rings are able to stack.
  - Atoms remain in contact more than in more flexible alkanes.
  - Molecules harder to separate – harder to boil (evaporate).
Properties of Cycloalkanes

Solubility
- What determined the solubility of alkanes in water?
- Do you think cycloalkanes will be different?

Cyclohexanes: examples
- Alkane products contain mixture that include cycloalkanes
  - Mineral oil
- Many biomolecules contain fused rings
  - Steroids
    - What kinds of rings are present?

Cycloalkanes: steroids
Hydrocarbons and your skin

- Oils
  - "waterproof" – prevent water from leaving the skin
  - Use after showering to "seal" in water
  - Petroleum jelly, mineral oil, lanolin
- Humectants
  - Attract water
  - Glycerol, lactic acid, propylene glycol

Chapter 12: Unsaturated Hydrocarbons

Alkenes, Alkynes, and Aromatics

So what’s the difference between saturated and unsaturated fats? And what exactly are these trans-fats?

It all has to do with hydrocarbons!

Objectives

- Recognize functional groups of alkenes, alkynes, and aromatics.
- Identify the geometry of carbons in each functional group.
- Name unbranched alkenes and alkynes.
- Identify the cause of cis trans isomerism and what molecules can display it.
- Identify and distinguish cis-trans isomers.
- Describe the effects of cis-trans isomerism on physical properties of alkenes.
- Describe the cause of stability of aromatic compounds.
- Identify PAHs.
- Identify the benzene ring used as a substituent.
- Recognize para, ortho, and meta substituents.

Suggested Problems Ch 12: 1-3a, 4a, 5a,b 7-12, 25, 28a,b, 39-41d,f, 42b,c,e, 43
**Alkenes**

- **Alkene**: A hydrocarbon that contains one or more carbon-carbon double bonds
  - Unsaturated
  - Ethene is the simplest alkene
    - Common name: Ethylene
  - How many hydrogens are attached to each C?
  - How many electrons do the carbons share?
    - Where are they located?

**Structure:**
- Planar molecule
- Approximately 120° bond angle around C
- No rotation around double bond

**Cis-trans isomerism**
- Because of restricted rotation about a carbon-carbon double bond, an alkene with two different groups on each carbon of the double bond shows cis-trans isomerism

**Examples:**
- **cis-2-Butene**: mp -139°C, bp 4°C
- **trans-2-Butene**: mp -106°C, bp 1°C
Cis-trans isomers

- **Cis** – the large groups are on the same side of the double bond
  - For the molecules we look at, this will put hydrogens on the same side of the double bond
- **Trans** – large groups (as well as hydrogen) are on opposite sides of the double bond

Which isomer is shown?

\[ \text{H}_2\text{C} - \text{C} - \text{H} \]
\[ \text{H} \quad \text{CH}_3 \]

Draw the other isomer.

Cis-Trans Isomerism

- Does the molecule to the right display cis-trans isomerism?

\[ \text{H}_2\text{C} - \text{C} - \text{H} \]
\[ \text{H} \quad \text{CH}_3 \]
\[ \text{CH}_3 \]

Cis-Trans in Long Chains

- Cis or Trans double bonds in long hydrocarbon chains give a characteristic appearance
- Label each as cis or trans and describe the difference between the two.

\[ \text{H}_2\text{C} - \text{C} - \text{C} - \text{C} - \text{H}_3 \]
\[ \text{H}_2\text{C} - \text{C} - \text{C} - \text{C} - \text{CH}_3 \]
Cis-Trans Isomers

- Fatty Acids
  - Fatty acids have long hydrocarbon chains
  - Melting point of hydrocarbons determined by amount of interactions between chains
    - Closely packed – many interactions – _________ mp
    - Bent chains – fewer interactions – _________ mp
  - Saturated chains – extended, many interactions
  - Trans chains – act like saturated - extended
  - Cis chains – bend, kink

Cis Fatty Acid structure

- Oleic Acid
- Linoleic acid

Cis-trans Fatty acids

- Safflower acid, a unsaturated fatty acid
- Octadecanoic acid

Triene acid, a polyunsaturated fatty acid
Both double bonds are cis
Fatty Acids

- **Saturated** hydrocarbons chains, and chains with **trans** bonds have _________ melting points than those with **cis** bonds

- Which fatty acids are solid at higher temperatures?

Alkynes

- **Alkyne**: a hydrocarbon that contains one or more carbon-carbon triple bonds
  - Ethyne is the simplest alkyne
    - Common name: acetylene
  - Where are the electrons in the triple bond located?

    ![Acetylene](image)

    Acetylene (an alkyne)

Alkynes: Structure

- A triple bond is linear.
- There is no rotation.
- Can there be cis-trans isomerism?
Alkenes /Alkynes- IUPAC Names

1. Name the parent chain: the longest chain that contains the multiple bond.
   - Use the ending -ene to show the presence of the C=C.
   - Use the ending -yne to show the presence of C≡C
2. Number the chain from the end that gives the lower numbers to the carbons of the C=C
3. Indicate the multiple bond by the number of its first carbon.
   - label cis/trans if applicable

CH₃CH₂CH₂CH₃CH=CH₂
1-Hexene

Does 1-hexene display cis-trans isomerism?

Nomenclature

- Name the compounds below
  H₂C═CH₂
  HC≡CH

Alkenes – IUPAC names

Name the compounds below:
H₃C
CH₃
H₃C
CH₃
**Alkynes – IUPAC Names**

- CH$_3$CH=CHCH$_2$CH$_3$

  - Remember that the triple bond is linear!
  - There are no bends in the bonds coming off the carbons!

**Cycloalkenes**

- To name a cycloalkene
  - Number the carbon atoms of the ring double bond 1 and 2 in the direction that gives the lower number to the substituent encountered first.
  - Number and list substituents in alphabetical order.

  - 3-Methylcyclopentene (not 5-methylcyclopentene)
  - 4-Ethyl-1-methylcyclohexene (not 5-ethyl-2-methylcyclohexene)

**Multiple multiple bonds!**

- You don't have to be able to name these, just recognize how many of what kind of bond are present!

  - Alkenes that contain more than one double bond are named as -dienes, -triens, and so on.
  - Alkynes with more than one triple bond are – diynes, triynes, etc.

  - 1,4-Pentadiene
  - 2-Methyl-1,3-butadiene
  - 1,3-Cyclopentadiene
Multiple Multiple bonds!

- If a compound contains both double and triple bonds it is named an enyne.
  - Number from end closest to first multiple bond.
  - If same for both, give double bond precedence

![Multiple bond example](image)

Unsaturated Hydrocarbons

Properties

- Nonpolar, so similar to alkanes
  - Insoluble in water
  - Soluble in other hydrocarbons
  - Less dense than (float on) water
  - Melting point determined by contact between atoms of different chains
    - Many contacts – higher melting point
      - Pack together well
      - Longer chains

Examples: Cis-Trans Isomers

Vitamin A and vision

- Cis – retinal
  - Made from vitamin A
- Used in cones for vision
- Conversion from cis to trans changes shape of molecule
  - Generates neuron pulse
Alkanes, Alkenes, Alkynes

- **Aliphatic**
  - General term for alkanes, alkenes, alkynes
  - from Greek for “fat”

- **Aromatic** - next section
  - Special arrangement of double bonds

Aromatic Compounds

- **Aromatic compound**: a hydrocarbon that contains one or more benzene-like rings
  - arene: a term used to describe substituted benzene compounds (as alkane, alkene, alkyne)
**Aromatic Compounds**

- Originally, aromatic was coined because of the smell of compounds.
- Not all aromatic compounds are fragrant.
- Aromatic now refers to the ring of alternating double bonds.

![Structure of aromatic compounds]

**Aromatic Compounds**

- The alternating bonds give aromatic compounds stability.
  - The alternating double bonds are spread out over the whole ring.
  - Less reactive than alkenes and alkynes.

![Additional structures of aromatic compounds]

**Properties of Aromatics**

- Higher boiling points than unsaturated counterparts
  - Flat, symmetric
  - Able to stack together – more interactions
- Density
  - Less than water
  - Greater than other hydrocarbons
- Solubility
  - What do you think, based on the chemical makeup?
Nomenclature

- monosubstituted alkylbenzenes are named as derivatives of benzene; for example, ethylbenzene
- the IUPAC system retains certain common names for several of the simpler monosubstituted alkylbenzenes;

CH₂CH₃

CH₃

CH=CH₂

OH

Ethylbenzene

Toluene

Styrene

Phenol

Nomenclature

- When there are two substituents on a benzene ring, the common name uses prefixes ortho, para, and meta to describe the positions relative to one another:
  - ortho (o) – _________ substituents
  - meta (m) - _________ substituents
  - para (p) - _________ substituents

Nomenclature

- Classify each as ortho, meta, or para:

CH₃

H₃C

H₂C

H₂C

Cl

Cl

CH₃

Cl

Cl

CH₃
Nomenclature

- If the benzene ring is attached to a more complex molecule it is named as a substituent.
- **Phenyl group**
  - \((\text{C}_6\text{H}_5\text{ or Ph})\): the substituent group derived by loss of an H from benzene

Toxicity: Benzene

- Benzene and other aromatic compounds are carcinogenic.
- **Benzene in soft drinks:**
  - Benzoate salts + vitamin C + high T can produce benzene in soft drinks.
  - U.S. benzene threshold for drinking water: 5 ppb
  - Some experiments showed 4 ppb in soft drinks studied
  - Some methods gave 23 ppb

PAHs

- **Polynuclear aromatic hydrocarbon (PAH)**
  - A hydrocarbon that contains two or more benzene rings, with each pair of rings sharing two adjacent carbon atoms
- **Toxicity**
  - Some are carcinogenic
    - Tobacco smoke, auto exhaust, charred food
  - Benzene itself is carcinogenic
  - Other PAHs are toxic to some extent

Toxicity: PAHs

- Some are carcinogenic
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![PAHs Diagram](image)
Some interesting compounds with phenyl rings.

Pseudoephedrine

Diphenhydramine

Loratidine

Some painkillers

Naproxen

Aspirin

Acetaminophen