

## **Chemistry 500: Chemistry in Modern Living**

### **Topic 7: Manipulating Molecules and Designing Drugs**

#### **Organic Chemistry**

Chemistry in Context, 2<sup>nd</sup> Edition: Chapter 11, Pages 351-386

Chemistry in Context, 3<sup>rd</sup> Edition: Chapter 10, Pages 375-414

Outline Notes by Dr. Allen D. Hunter, YSU Department of Chemistry, ©2000.

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## 7A Organic Chemistry

- Organic Chemistry is the study of the **chemistry of carbon**
  - What makes carbon special?
    - Many **bond types**
    - Forms long **chains**
    - Forms **strong bonds** to almost all elements
  - Over 16,000,000 organic compounds known
  - Being discovered at the rate of over 1,000,000 per year
  
- **Bonding**
  - **Lewis dot structures**
    - Remember from Topic 2 the ways that different elements  
bond

- **Bond Distances and Bond Angles**
  - **Ethane, C<sub>2</sub>H<sub>6</sub>**
    - **Carbon - Carbon Single Bond**
    - **C-C distance of 1.54 Å**
    - **Bond angles of 109.5 °**
  
  - **Ethene, C<sub>2</sub>H<sub>4</sub>**
    - **Carbon - Carbon Double Bond**
    - **C-C distance of 1.34 Å**
    - **Bond angles of 120 °**
  
  - **Ethyne, C<sub>2</sub>H<sub>2</sub>**
    - **Carbon - Carbon Single Bond**
    - **C-C distance of 1.20 Å**
    - **Bond angles of 180 °**

## 7B How Do We Know Molecular Structures?

- First Approach
  - Logical Reasoning
    - Informed by reactivities and crude compositions
    - Only tools available were:
      - Balances
      - Melting Points, mp
      - Boiling Points, bp
      - Taste, Smell, Textures, etc.

➤ Second Approach

➤ Elemental Analysis

➤ Classical Wet Methods

➤ One element at a time

➤ Example:  $\text{Ag}^+$  precipitation of  $\text{Cl}^-$

➤ Instrumental Methods

➤ Multi-element Simultaneous

➤ Automated

➤ Example: Combustion Analysis

➤ Third Approach

➤ X-Ray Diffraction

➤ What is a **crystal**?

➤ What is an **X-ray**?

➤ What are the components of a **diffractometer**?

➤ How does one solve a structure?

➤ Types and Reliability of Information

➤ Fourth Approach

➤ Sporting Methods

➤ The specific absorption of electromagnetic waves

➤ The pattern of the absorption tells us information about the structure (indirectly)

➤ Infrared Spectroscopy, IR

➤ Ultraviolet-Visible Spectroscopy, UV-Vis

➤ Nuclear Magnetic Resonance Spectroscopy, NMR

➤ Mass Spectroscopy, MS



7C Approaches to Making Molecules

➤ Synthetic Methods Development

➤ Conventional Serial Synthesis Methods

➤ Combinatorial Synthesis Methods

## 7D Structural Isomers

- Definition
  - Same atoms but attached differently
  
- Types
  - Positions of Atoms
  - **Strait Chain** vs. **Branched Chain**
  - **Multiple Bonds** vs. **Rings**
  
- Example [For the following molecular formulae, draw all of the structural isomers (up to a maximum of 5). Be sure that you show **all** atoms and bonds for each.]
  - $C_2H_6O$

➤ Ask Students: For each of the following molecules, draw all structural isomers (up to a maximum of five)

➤ Group Activity

➤  $C_2H_6O_2$

➤  $C_3H_9N$



## 7E Functional Groups

➤ Graphics from Text: Figure 11.2 in 2<sup>nd</sup> Edition and 10.2 in 3<sup>rd</sup>

Edition, Functional Group Classification

➤ Hydrocarbons

➤ Alkanes

➤ Alkenes

➤ Alkynes

➤ Arenes

➤ Groups with Oxygen(s)

➤ Alcohols

➤ Ethers

➤ Aldehydes

➤ Ketones

➤ Carboxylic Acids

➤ Esters



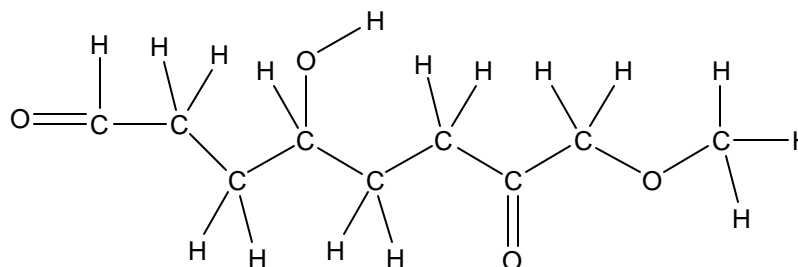
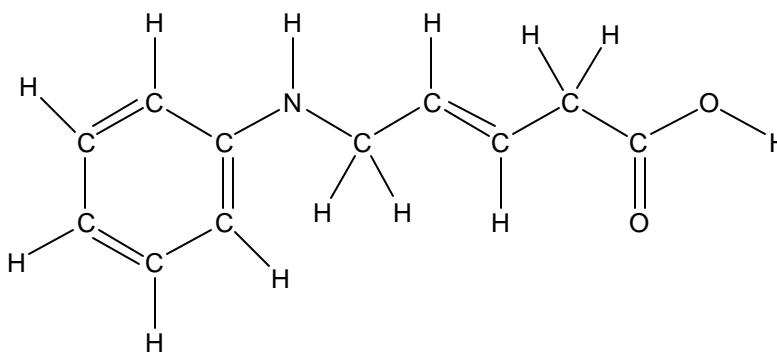
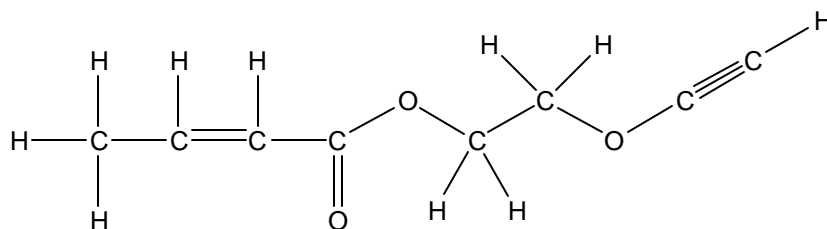
➤ Groups with Nitrogen

➤ Amines

➤ Amides

➤ Ask Students: In the following molecule(s), identify all functional groups by circling them and then name each functional group

➤ Group Activity



➤ Asks Students: Draw a molecule with each of the following functional groups (making sure to label each)

➤ Group Activity

➤ Alcohol, Alkene, and Ether

➤ Arene, Amine, and Ketone

➤ Carboxylic Acid, Alkyne, and Ester

## 7F Drug Discovery

- Sources of potential pharmaceuticals
  - Natural products isolation
  
  - Biochemical understanding
  
  - Random Synthesis
    - Synthetic molecules
  
    - Semisynthetic molecules

- Process of drug discovery
  - Approximately 10,000 chemicals screened for every new product
  
  - Typically it costs between \$300,000,000 to \$500,000,000 to bring a new **drug candidate to market**
  
  - Stages
    - Initial candidate drug discovery
    - Study of **biochemistry / physiology / pharmacology**
    - **Systematic variation of drug structure**
    - **Scale up of production**
    - **Marketing**
    - Throughout: **safety and efficacy testing**

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