

Chemistry 500: Chemistry in Modern Living

Topic 7: Manipulating Molecules and Designing Drugs

Organic Chemistry

Chemistry in Context, 2nd Edition: Chapter 11, Pages 351-386

Chemistry in Context, 3rd 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_2H_6
 - Carbon - Carbon Single Bond
 - C-C distance of 1.54 Å
 - Bond angles of 109.5°

 - Ethene, C_2H_4
 - Carbon - Carbon Double Bond
 - C-C distance of 1.34 Å
 - Bond angles of 120°

 - Ethyne, C_2H_2
 - 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: Ag^+ precipitation of 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

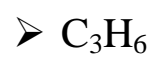
- Example [For the following molecular formulae, draw all of the structural isomers (up to a maximum of 5). Be sure that you show **all** atoms and bonds for each.]
 - C_2H_6O

➤ 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



➤ Alkynes

➤ Arenes

➤ Groups with Oxygen(s)

➤ Alcohols

➤ Ethers

➤ Aldehydes

➤ Ketones

➤ Carboxylic Acids

➤ Esters

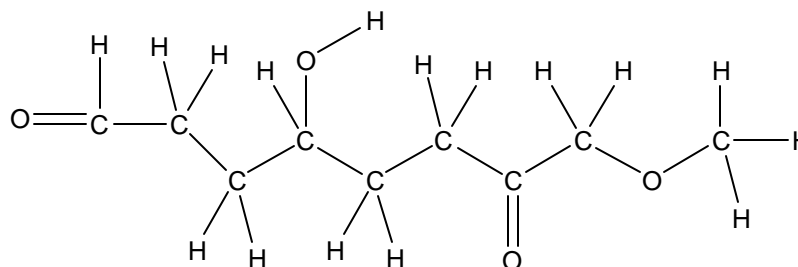
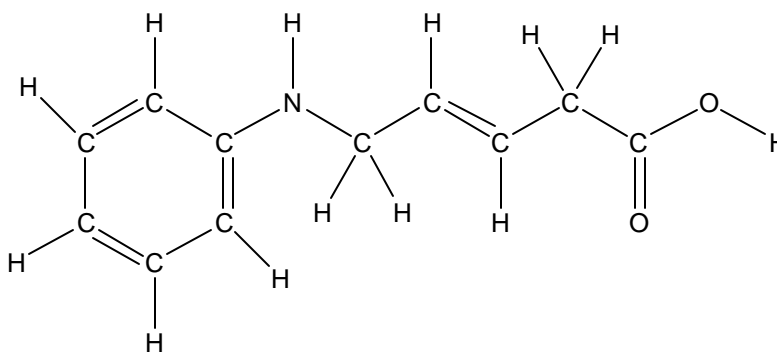
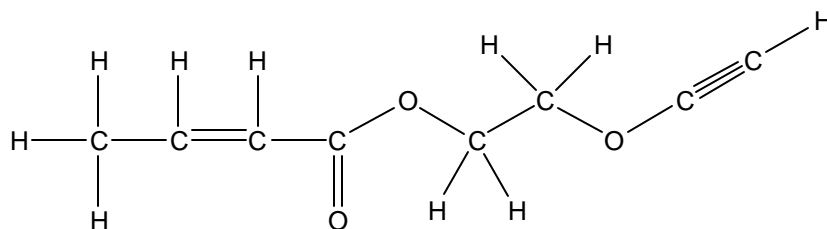
➤ Groups with Nitrogen

➤ 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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120 °	4
180 °	4

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