Chemistry 1500: 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
Chemistry in Context, 4th Edition: Chapter xxx, Pages xxx-xxx

The Figure, Table, & Problem numbers in these notes are taken from the 4th edition of the text unless otherwise noted.

Graphics from Text: Figure xxx.0
Outline

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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, C₂H₆**
  - Carbon - Carbon Single Bond
  - C-C distance of 1.54 Å
  - Bond angles of 109.5 °

- **Ethene, C₂H₄**
  - Carbon - Carbon Double Bond
  - C-C distance of 1.34 Å
  - Bond angles of 120 °

- **Ethyne, C₂H₂**
  - 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: $\text{Ag}^+ \text{ precipitation of } \text{Cl}^-$

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.]

➤ C₂H₆O
➢ Ask Students: For each of the following molecules, draw all structural isomers (up to a maximum of five)

➢ Group Activity

➢ C₂H₆O₂

➢ C₃H₉N
\[ \text{C}_4\text{H}_{10} \]

\[ \text{C}_3\text{H}_6 \]
7E Functional Groups

- Graphics from Text: Figure 11.2 in 2nd Edition and 10.2 in 3rd 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

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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
# Index of Vocabulary and Major Topics

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