Chemistry 500: Chemistry in Modern Living

Topic 7: Manipulating Molecules and Designing Drugs

Organic Chemistry

Chemistry in Context, 2\textsuperscript{nd} Edition: Chapter 11, Pages 351-386

Chemistry in Context, 3\textsuperscript{rd} Edition: Chapter 10, Pages 375-414

Outline Notes by Dr. Allen D. Hunter, YSU Department of Chemistry, ©2000.
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: $\text{Ag}^+$ 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.]

- \( \text{C}_2\text{H}_6\text{O} \)
Ask Students: For each of the following molecules, draw all structural isomers (up to a maximum of five)

- Group Activity

- $\text{C}_2\text{H}_6\text{O}_2$

- $\text{C}_3\text{H}_9\text{N}$
\[
\text{C}_4\text{H}_{10}
\]

\[
\text{C}_3\text{H}_6
\]
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
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
**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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