

## Chemistry 506: Allied Health Chemistry 2

### Chapter 10, Structure and Bonding in Alkanes

#### Basics of Structure and Bonding

Introduction to General, Organic & Biochemistry, 5<sup>th</sup> Edition by  
Bettelheim and March: Chapter 10, Pages 309-352

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## 10A Section(s) 10.1 What is an Organic Chemical?

- Definition
  - Compounds of Carbon
  - Mostly Covalent Bonding
  - Related to Molecules of Life
  
- Where do they come from?
  - Numbers
    - Total (> 10,000,000)
      - Fully isolated, characterized, and reported
    - New (> 500,000 / year)
    - Accelerating rate of discovery
      - Linear Synthetic Strategies vs. Combinatorial Synthetic Strategies
      - Characterization Methods
      - Automation and Productivity

- What is so Special about Carbon?
  - Bond Orders (single bonds, double bonds, and triple bonds)
  - Strong Stable bonds to almost all atom types
  - Long chains
  - This is a unique combination

## 10B Section(s) 10.2 Sources of Organic Carbons

- Nature and Organic Chemicals
  - Isolation from natural sources
  - natural products
  
- Synthesis and Organic Chemicals
  - man made organic products
  - lab scale synthesis vs. factory scale synthesis
  
- Production Choices from Dual sources
  - Cost Considerations and environmental considerations
  
- Semi-Synthetic Organic Compounds

## 10C Section(s) 10.3/4 Structures and Bonding

- How Do We Know Structures?
  - Analytical Data
  
  - Spectroscopic Methods
    - Sporting Methods
    - Specific absorption of light
    - NMR = Nuclear Magnetic Resonance (cf. MRI, Magnetic Resonance Imaging)
    - Infra-Red (IR)
    - Ultra Violet-Visible (UV-Vis)

- **X-Ray Crystallography/Diffraction**
  - Non-Sporting Method
  - **Single Crystals**
  - Hardware
  - Data Collection
  - Data Analysis
  
- **General Features of Structures**
  - **Complex 3D Shapes**
    - **109.5°, 120°, and 180° Bond Angles**
    - **1.2 – 1.55 Å Bond Distances (C-H ≈ 1 Å)**
  - **Structural Correlations with Properties**

➤ **Molecular Formulae**

➤ Elements present

➤ Number of atoms of each type

➤ **Molecular Weight**

➤ Not unique to molecules

➤ e.g.  $C_{11}H_{14}O$

- **Structural Formulae**
  - Connectivity
  - 3D Structures (unique)
  - Related to **Properties**
    - **Mp, Bp, taste, toxicity, strength, etc.**
  - Examples a few pages on



- Rationalization by Lewis, VSEPR, and VBT Theories
  - Lewis Theory Review (section 3.6)
    - Lone pairs and bonds
    - Valence electrons
  - Rigorous Method
    - Count number of valence electrons
    - Place total number of valence electrons around each atom to give it a complete octet

- Quick and dirty Lewis method (for common "organic" elements)
- Bond Lengths
- Bond Angles

H  $\Rightarrow$  one bond and no lone pairs

F, Cl, Br, and I  $\Rightarrow$  one bond and three lone pairs

O, S, Se, and Te  $\Rightarrow$  two bonds and two lone pairs

N, P, As, and Sb  $\Rightarrow$  three bonds and one lone pair

C, Si, Sn, and Ge  $\Rightarrow$  four bonds and no lone pairs

➤ VSEPR, Valence Shell Electron Pair Repulsion Theory,

Review

- Molecular shapes  $\Rightarrow$  bond angles
  - Four groups  $\Rightarrow$  Tetrahedral, td
  - Three groups  $\Rightarrow$  Trigonal planar
  - Two groups  $\Rightarrow$  Linear
  
- Number of "things"
  - 4 things  $\rightarrow 109.5^\circ$
  - 3 things  $\rightarrow 120^\circ$
  - 2 things  $\rightarrow 180^\circ$

➤ Valence Bond Theory, VBT, Review

➤ Hybridization

➤  $109.5^\circ \rightarrow sp^3$

➤  $120^\circ \rightarrow sp^2$

➤  $180^\circ \rightarrow sp$

- Examples of Problem Types
  - Predict **Lewis Structures**
  - Predict **hybridizations**
  - Predict **bond angles**
  - Predict **bond lengths**
  
- **Worked Example(s)** [For each of the following molecules, draw the correct Lewis structure and predict the hybridizations, bond lengths and bond angles around the \* atoms.]

➤ **Structural Isomers**

➤ Definition

➤ Same atoms but attached differently

➤ Types

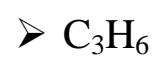
➤ Positions of Atoms

➤ **Strait Chain** vs. **Branched Chain**

➤ **Multiple Bonds** vs. **Rings**

➤ **Examples** [For 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.]

➤  $C_2H_6O$



## 10D Section(s) 10.5/6 Hydrocarbons and Alkanes

### ➤ Definitions

#### ➤ Hydrocarbon

➤ ( $C_nH_m$ )

➤ sources

#### ➤ Alkane

➤ ( $C_nH_{2n+2}$ , e.g.,  $C_2H_6$ ,  $C_5H_{12}$ ,  $C_{100}H_{202}$ )

➤ only **single bonds**

#### ➤ Alkene

➤ At least one **double bond**

#### ➤ Alkyne

➤ At least one **triple bond**

#### ➤ Aromatic/Arene

➤ "**benzene like**"

➤ "alternating" single and double bonds around a ring



- Examples of Alkanes
  - Methane (sources, cost),  $\text{CH}_4$
  
  - Ethane,  $\text{C}_2\text{H}_6$
  
  - Propane,  $\text{C}_3\text{H}_8$
  
  - Butane,  $\text{C}_4\text{H}_{10}$
  
  - **Know C1-C10 Alkane Names** (Table 10.4) (**Pent, Hex, Hept, Oct, Non, Dec**)
  
  - **Molecular Weight -> Mp and Bp**

- Structures of Alkanes
  - Bond angles ( $\approx 109.5^\circ$ )
  - Bond distances ( $\approx 1.54 \text{ \AA}$  (C-C) and  $1.0 \text{ \AA}$  (C-H))
  - Ring Strain (C3 and C4 rings)
  
- Types of Carbons in Alkanes
  - $1^\circ$ , Primary Carbon,  $\text{CH}_3$
  - $2^\circ$ , Secondary Carbon,  $\text{CH}_2$
  - $3^\circ$ , Tertiary Carbon,  $\text{CH}$
  - $4^\circ$ , Quaternary Carbon,  $\text{C}$
  - Examples

- **Rotation Around Bonds in Alkanes**
  - **$\sigma$ -Bonds, Sigma-Bonds**
  - **Free Rotation or Restricted Rotation?**
  - **Steric Effects, Rings**
  
- **Alkane Structural Isomers**
  - **e.g. C5**

## 10E Section(s) IUPAC Nomenclature

- Steps
  - Find **longest continuous chain** (Alkane)
  - **Number carbons in chain** from end that give side chains  
lowest number
  - Identify **side chains**
    - Name
    - **Attachment Position(s)**
    - **Number of groups** (di, tri, tetra, penta, hexa, hepta, octa, nona, deca)
  - Assemble name (**punctuation**)
    - ,
    - -

- Side Chain Names
  - Alkyl (Table 10.4 for prefixes)
  
  - Methyl,  $\text{CH}_3$
  
  - Ethyl ( $\text{C}_2\text{H}_5$ )
    - $\text{CH}_2\text{CH}_3$
  
  - Propyl ( $\text{C}_3\text{H}_7$ )
    - n-propyl
    - iso-propyl
  
  - Butyl ( $\text{C}_4\text{H}_9$ )
    - n-butyl
    - iso-butyl
    - sec-butyl
    - tert-butyl

- Pentyl, etc.
  - n-alkyl
  - Iso-alkyl
  
- Halogens
  - Fluoro
  - Chloro
  - Bromo
  - Iodo
  
- Examples

10F Section(s) Cycloalkanes

- cyclo prefix
  - cyclobutane, cyclohexane, etc.
  - number from functional groups
  
- Ring strain (C3 & C4)
  
  
- Examples

10G Section(s) 10.7 Skip

10H Section(s) 10.8 Physical Properties

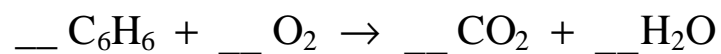
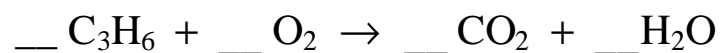
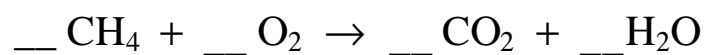
- Physical State
  - Mp and Bp
  - Depends on MW
  - Van der Waals Forces
  - Intermolecular Bonding vs. Intramolecular Bonding
  
- Non-Polar compounds
  - Definition of Polar vs. Non-Polar
  
- Solubility
  - Non-polar organic solvents vs. water
  
- Density
  - Cf. water



10I Section(s) 10.11 Chemical Properties

➤ UNREACTIVE

➤ Combustion (balance reactions)



10J Section(s) 10.12 Functional Groups

➤ Framework vs. Functional Group

➤ Identifying Functional Groups

➤ Table 10.7, p342

➤ Alkene

➤ Alkyne

➤ Aromatic

➤ Alkyl Halide

➤ Alcohol

➤ Ether

➤ Thiol (mercaptan)

➤ Amine

➤ Aldehyde

➤ Ketone

➤ Carboxylic Acid

➤ Ester

➤ Amide

**Problems** 10.1 – 10.51 (except 10.36 b, c, f, and 10.37)

10K Section(s) 18.2 Amino Acids having Alkyl Side Chains

- Amino Acids (Building Blocks of Proteins)
- Generic AA =  $\text{H}_2\text{N}-\text{CHR}-\text{CO}_2\text{H}$
  
- 6 Nonpolar Alkyl Side Chains
  
- Glycine, R = H
  
- Alanine, R =  $\text{CH}_3$ , methyl
  
- Valine, R =  $\text{CH}(\text{CH}_3)_2$ , isopropyl
  
- Leucine, R =  $\text{CH}_2\text{CH}(\text{CH}_3)_2$ , isobutyl
  
- Isoleucine, R =  $\text{CH}(\text{CH}_3)(\text{CH}_2\text{CH}_3)$ , sec-butyl
  
- Proline,  $\text{HN}\{\text{CH}_2\text{CH}_2\text{CH}_2\text{-ring}\}\text{CH}-\text{CO}_2\text{H}$

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