

## Chemistry 1506: Allied Health Chemistry 2

### Section 1: Structure and Bonding in Alkanes

#### Basics of Structure and Bonding

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## Section 1.1 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 (> 1,000,000 / 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

## Section 1.2 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

## Section 1.3 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**
    - C~C Distances: 1.2 – 1.55 Å **Bond Distances** for Hydrocarbons and  $\approx 1.54$  Å for Alkanes (and C-H  $\approx 1$  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

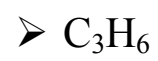
➤  $109.5^\circ$  ->  $sp^3$

➤  $120^\circ$  ->  $sp^2$

➤  $180^\circ$  ->  $sp$

- 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.]
    - $C_2H_6O$



## Section 1.4 Hydrocarbons and Alkanes

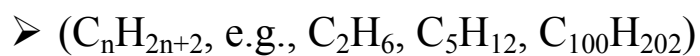
### ➤ Definitions

#### ➤ Hydrocarbon



➤ sources

#### ➤ Alkane



➤ 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** (See Table in Text) (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. C<sub>5</sub>

## Section 1.5 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** (See Table in text 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

## Section 1.6 Cycloalkanes

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

## Section 1.7 Physical Properties

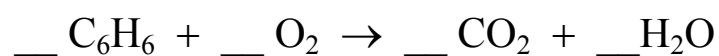
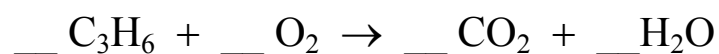
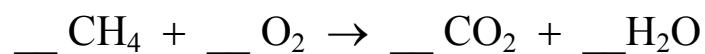
- Physical State
  - Mp and Bp
  - Depends on MW
  - Van der Waals Forces
  - Intermolecular Bonding vs. Intramolecular Bonding
  
- Non-Polar compounds
  - Definition of Polar vs. Non-Polar
  
- Solubility
  - Non-polar organic solvents vs. water
  
- Density
  - Cf. water



**Section** 1.8 Chemical Properties

➤ UNREACTIVE

➤ Combustion (balance reactions)





➤ Ether

➤ Thiol (mercaptan)

➤ Amine

➤ Aldehyde

➤ Ketone

➤ Carboxylic Acid

➤ Ester

➤ Amide

## Section 1.10 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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