Chemistry 1506: Allied Health Chemistry 2

Section 1: Structure and Bonding in Alkanes

Basics of Structure and Bonding

Outline

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 ≈ 1.54 Å for Alkanes (and 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 ⇒ bond angles
    - Four groups ⇒ Tetrahedral, td
    - Three groups ⇒ Trigonal planar
    - Two groups ⇒ Linear

- Number of "things"
  - 4 things -> 109.5°
  - 3 things -> 120°
  - 2 things -> 180°

- Valence Bond Theory, VBT, Review
  - Hybridization
  - 109.5° -> sp^3
  - 120° -> sp^2
  - 180° -> 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

C_4H_{10}

- C_3H_6

Section 1.4 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), CH_4
  - Ethane, C_2H_6
  - Propane, C_3H_8
  - Butane, C_4H_{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 (≈ 109.5°)
  - Bond distances (≈ 1.54Å (C-C) and 1.0Å (C-H))
  - Ring Strain (C3 and C4 rings)

- Types of Carbons in Alkanes
  - 1°, Primary Carbon, CH_3
  - 2°, Secondary Carbon, CH_2
  - 3°, Tertiary Carbon, CH
  - 4°, Quaternary Carbon, C
  - Examples

- Rotation Around Bonds in Alkanes
  - σ-Bonds, Sigma-Bonds
  - Free Rotation or Restricted Rotation?
  - Steric Effects, Rings

- Alkane Structural Isomers
  - e.g. C5

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, CH_3
  - Ethyl (C_2H_5)
    - CH_2CH_3
  - Propyl (C_3H_7)
    - n-propyl
    - iso-propyl
  - Butyl (C_4H_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)

$$\_\_\ CH_4 + \_\_\ O_2 \rightarrow \_\_\ CO_2 + \_\_H_2O$$

$$\_\_\ C_3H_6 + \_\_\ O_2 \rightarrow \_\_\ CO_2 + \_\_H_2O$$

$$\_\_\ C_6H_6 + \_\_\ O_2 \rightarrow \_\_\ CO_2 + \_\_H_2O$$

Section 1.9 Functional Groups

- Framework vs. Functional Group
  - Identifying Functional Groups
  - (See Table in text for Functional Groups)
- Alkene
- Alkyne
- Aromatic
- Alkyl Halide
- Alcohol

- 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 = $H_2N\text{-}CHR\text{-}CO_2H$
- 6 Nonpolar Alkyl Side Chains
- Glycine, R = H
- Alanine, R = CH_3, methyl
- Valine, R = $CH(CH_3)_2$, isopropyl
- Leucine, R = $CH_2CH(CH_3)_2$, isobutyl
- Isoleucine, R = $CH(CH_3)(CH_2CH_3)$, sec-butyl
- Proline, $HN\{CH_2CH_2CH_2\text{-ring}\}CH\text{-}CO_2H$

Index of Topics and Vocabulary