

Chapter 1 Lecture Outline **Introduction to Structure and Models of Bonding**

assigned problems: 1-2, 5-6, 9-11, 13, 16-17, 19, 21-22, 24, 28-29, 32-33

Key Concepts and Learning Goals

- be able to write complete Lewis structures for organic molecules
- be able to identify the local orbital structure for valence electrons in any Lewis structure
- be able to write resonance structures for molecules and evaluate their relative importance
- write Lewis-Linnett structures of molecules with odd electron bonds
- be able to predict the atom geometry in organic structures from Lewis structures
- identify pi systems and # pi electrons in molecules
- know relative atom electronegativities, polarizabilities, van der Waal radii, and avg C-C bond length and strength
- predict bond polarity and relative molecule dipole moments
- be able to construct group orbitals for methyl, methylene, and related common organic substructures
- write pi MO diagrams for organic pi systems
- be able to evaluate molecular structure and reactivity based on an orbital deconstruction of molecular electron density

I. Atomic Orbitals, Atom Hybridization, and Molecular Geometry

- A. quantum numbers and atomic orbital functions
- B. atom electron configuration - ground states and excited states and Hund's rule
- C. sigma and pi bonding, atom hybrid orbitals, and atom geometry in molecules

II. Lewis Structures of Organic Molecules - a valence bond approach

- A. Lewis structures: show all valence electrons, obey octet rule, include formal charges, include resonance structures as needed
- B. identifying conjugated pi-systems
- C. cases when pi-electron delocalization does not occur in molecules with contiguous p-orbitals
- D. Lewis-Linnett structures and odd-electron bonds

III. Atom Electronic Properties and Effects on Molecular Structure

- A. atom and group electronegativities and bond polarity
- B. bond and molecule dipole moments
- C. atom sizes, bond lengths, and molecular dimensions
- D. atom and molecule polarizability

IV. Molecular Orbital Theory and Common Group Orbitals

- A. introduction to MO theory of organic molecules
 1. the Schrodinger Equation
 2. the total wave function and its square
 3. a molecular orbital and the LCAO approximation
- B. pi-system MOs
 1. linear pi systems
 2. cyclic pi systems
- C. symmetry adapted orbitals - delocalized sigma bonds
 1. molecular symmetry and symmetry terms
 2. CH₃ group orbitals
 3. CH₂ group orbitals
- D. ethane, ethene, and formaldehyde orbital structure and their FMOs
- E. summary of basic tenants of qualitative molecular orbital theory

V. Orbital Structure of Reactive Intermediates and Aromatic Structures

- A. hyperconjugation
- B. α -amino radicals and the 3-electron pi bond
- C. arenium cation intermediate in toluene ring bromination
- D. propene conformation