

Review Outline Midterms #1-#2 Weeks 1-6 Chemistry 1B-02, Fall 2016

----- Chapter 12 -----

I. Experiments and findings related to origin of quantum mechanics

- A. Planck: $E=h\nu$, $\lambda\nu=c$
- B. Davisson-Germer (electrons diffract; behave as waves)
- C. DeBroglie $p\lambda=h$
- D. Photoelectric effect
- E. Uncertainty Principle $(m\Delta u)(\Delta x) \geq h/4\pi$
- F. Meaning of the "electron wave"
- G. Bohr and Rydberg and hydrogen atom
 $[E=-2.18 \times 10^{-18} \text{ J } (1/n^2)]$
 $[\Delta E=h\nu=hc/\lambda= -2.18 \times 10^{-18} \text{ J } (1/n_1^2 - 1/n_2^2)] (n_2 > n_1)$

II. Quantum mechanics of the hydrogen atom

- A. Wavefunction for an electron (Ψ), probability (Ψ^2), and radial probability ($4\pi r^2\Psi^2$)
- B. Quantum numbers n , l , m_l of allowed orbitals
 1. $n = 1, 2, 3, \dots$
 2. $l = 0, 1, 2, \dots (n-1)$ [s, p, d, f, ...]
 3. $m_l = -l \dots +l$ [($2l + 1$) components (values of m_l) for each l]
- C. Pictures of the orbitals and nodes
 1. $(n-l-1)$ radial nodes
 2. l angular nodes
 3. s, p_x , p_y , p_z , d_{z^2} , $d_{x^2-y^2}$, d_{xy} , d_{xz} , d_{yz}
- D. Meaning of the n , l , m_l quantum numbers
 1. n - energy, radial nodes, average distance of electron from nucleus
 2. l - shape of orbital
 3. m_l - orientation of orbital

III. Many-electron atoms and ions

- A. Stern-Gerlach and electron spin ($m_s = +1/2 \uparrow$, $m_s = -1/2 \downarrow$)
- B. Pauli exclusion principle
- C. Z_{eff} and shielding by inner electrons and electrons in same shell
- D. $E \approx -2.18 \times 10^{-18} \text{ J } (Z_{\text{eff}}^2/n^2)$
- E. $r \approx (0.529 \times 10^{-10} \text{ m}) (n^2/Z_{\text{eff}})$
- F. Z_{eff} of 2s > Z_{eff} of 2p due to penetration
- G. $E_{2s} < E_{2p}$
- H. $E_{3s} < E_{3p} < E_{3d}$
- I. Mnemonic diagram for energy ordering in neutral atoms (e.g. $E_{4s} < E_{3d}$)
- J. In transition metal cations $E_{3d} < E_{4s}$ (Z_{eff} vs n)
- K. Aufbau principle, Hund's Rule, and atomic configurations
- L. Ground, excited, and not allowed configurations

To Here Midterm #1

IV. Periodic properties of atoms

- A. Z_{eff} increases as one goes across period
- B. n increases as one goes down a group
- C. $E \approx -2.18 \times 10^{-18} \text{ J } (Z_{\text{eff}}^2/n^2)$ $r \approx (0.529 \times 10^{-10} \text{ m}) (n^2/Z_{\text{eff}})$
- D. Concepts of ionization energy (IE) and electron affinity (EA)
- E. IE increases across a period, decreases down a group
- F. Atomic radius decreases across a period, increases down a group
- G. EA (magnitude) increases across a period (until inert gasses) and decreases down a group
- H. Z_{eff} for positive and negative ions, relative size and IE of positive and negative ions
- I. Higher ionization energies
 - 1. $\text{IE}_1 < \text{IE}_2 < \text{IE}_3 \dots$
 - 2. big jumps in IE_x when removing electrons from next inner shell (how to use configurations of ions to rationalize successive IE's)
- J. Metals and nonmetals in periodic table

----- Chapter 13 -----

V. General considerations regarding bonding in molecules

- A. G.N. Lewis and the origin of the octet argument
- B. Electronegativity and periodic trends in electronegativity (metallic and nonmetallic elements)
- C. What types of atoms form ionic, covalent, or metallic compounds
- D. Ionic compounds
 - 1. Which elements form ionic compounds
 - 2. Molecular formulas for ionic compounds based on periodic table [know polyatomic anions]
 - 3. Lattice energy and charge and size (distance) effects on trends in lattice energy
 - 4. Properties of ionic compounds [high boiling and melting; 'crack' or fracture; conduct electricity in molten (liquid) or in solution]
- E. Covalent compounds [strong intramolecular bond, weaker intermolecular ; low boiling and melting points; poor conductors]
- F. Polar bonds and electronegativity
- G. Metallic bonding [moderate melting points; malleable; conduct electricity]

VI. Classical theories of chemical bonding and geometry

- A. Lewis electron dot structures
 - 1. Octets
 - 2. Lone pairs
 - 3. Multiple bonds
 - 4. Resonance structures
 - 5. Exceptions (reason why some atoms can form 10, 12, 14 electron shells)
 - 6. Formal charge from Lewis structures
 - 7. Bond energy and bond length
- B. Valence State Electron Pair Repulsion theory (VSEPR)
 - 1. Basic concepts (how electron group arrangement is related to electronic geometry and molecular shape)
 - 2. How to determine number of electron groups (steric number, SN)

3. Arrangement of electron groups (electronic geometry) based on SN
4. Molecular shape (i.e. molecular geometry) based on electronic geometry and placement of lone pairs
5. Various molecular shapes and bond angles and effect of lone pairs on bond angles
6. Dipole moments in polyatomic molecules

----- Chapter14 -----

VII. Quantum mechanics of covalent bonding

- A. Constructive interference of a.o.s to gives bonding molecular orbital
 1. Bonding m.o. has lower energy than energy of constituent a.o.s
 2. Bonding mo gives larger electron density in region between nuclei than would the sum of noninteracting atomic orbitals
- B. Destructive interference of a.o.s gives antibonding molecular orbital
 1. Antibonding m.o. has higher energy than energy of constituent a.o.s
 2. Antibonding mo gives smaller electron density in region between nuclei than would the sum of noninteracting atomic orbitals (has a node in bonding region)
- C. σ and π m.o.s

VIII. Molecular orbitals for diatomic molecular orbitals

- A. General rules for when a.o.s combine to for m.o.s
 1. A.O.s must have similar energies
 2. A.O.s must have nonzero overlap; must be able to have net constructive or destructive interference
 3. Identification of "pictures" of m.o.s
- B. M.O.s and energy ordering for 2nd row homonuclear diatomics
 1. Simple scheme:

$\sigma_{1s}, \sigma^*_{1s}, \sigma_{2s}, \sigma^*_{2s}, \sigma_{2p}, \pi_{2p}, \pi^*_{2p}, \sigma^*_{2p}$; applies to O₂, F₂
 2. Complex scheme with 2s \leftrightarrow 2p mixing:

$\sigma_{1s}, \sigma^*_{1s}, \sigma_{2s}, \sigma^*_{2s}, \pi_{2p}, \sigma_{2p}, \pi^*_{2p}, \sigma^*_{2p}$; applies to B₂, C₂, N₂
- C. Aufbau principle and molecular properties for homonuclear diatomics and ions
 1. Write and/or identify ground, excited, impossible molecular orbital configurations
 2. Bond order, bond energy, and stability of molecule
 3. Unpaired electrons and paramagnetism or diamagnetism
 4. Know how bond order is related to vibrational frequency
- D. Additional considerations for heteronuclear diatomics

Same general principles as for homonuclear diatomics (see IX .A. above) but:

 1. Differing a.o.'s on two atoms may have similar energies (e.g. H1s and F2p in HF)
 2. A.O.s do not contribute equally
 - a. Lower energy a.o. contributes more to bonding m.o.
 - b. Higher energy a.o. contributes more to antibonding m.o.
 - c. Polar bonds arise from this unequal mixing

To Here Midterm #2