Chem-601: Structure and Bonding of Molecules and Materials

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Office: Chemistry 4101
Office hours: MW 2-3, and by appointment

Lectures: Chemistry 0122  
MWF, 10 AM – 10:50 AM

Grading scheme:  
- 8 problem sets  
- Midterm exams (2)  
- Final exam  
  TOTAL  
  150 points total  
  75 points each  
  100 points  
  400 points

Textbooks:  

Tentative lecture schedule (readings in parentheses):

1.) A survey of inorganic and materials chemistry today
2.) Atomic structure  
   a. Refresher on quantum and hydrogen-like orbitals (IC 2.1 to 2.2.2).  
   b. Multi-electron orbitals, aufbau principle, and periodicity (IC rest of Ch. 2).
3.) Simple bonding models in molecules and solids  
   a. Octet rule, VSPER structures, the valence bond model and resonance (IC Ch 3).  
   b. Ionic bonding, prototype solid structures, Born-Haber cycle to calculate lattice energies (IC 7.1 to 7.2.2).
4.) Group theory  
   a. Symmetry elements, point groups, and multiplication tables (MSGT Ch. 1).  
   b. Representations and character tables (MSGT Ch. 2).  
   c. Irreducible representations and correlation tables (MSGT Ch. 3)  
   d. Group theory approach to VB theory and hybrid orbitals (MSGT 4.1 to 4.2)
5.) Molecular orbital theory  
   a. Linear combination of atomic orbitals, homonuclear diatomic molecules (IC 5.1 to 5.2.5)  
   b. Polar and larger molecules (IC rest of Ch. 5).  
   c. Symmetry adapted linear combination (SALC) orbitals (MSGT 4.3 to 4.5).  
   d. SALCs and the projection operator (MSGT Ch. 5).
6.) MO approach to bonding in solids  
   a. Introduction to space groups and crystallography (IC 7.1 to 7.1.1)  
   b. Covalent bonding in solids, band theory, Pierls distortion (handouts)  
   c. Semiconductors, insulators, and metals (IC 7.3 to 7.4).  
   d. Transition metal oxides and superconductors (handouts).
7.) Acid-base chemistry  
   a. Arrhenius, Brönsted, and Lewis theories (IC 6.1 to 6.2.8).  
   b. Hard and soft acids and bases (IC 6.3).  
   c. Acid/base strength (IC rest of Ch. 6).
8.) Redox chemistry (handouts)  
   a. Reduction potentials in aqueous and nonaqueous solvents.  
   b. Latimer, Frost, and Pourbaix diagrams.
9.) Methods of characterization in inorganic chemistry (handouts)
   a. Diffraction and spectroscopy including X-rays, neutrons, IR, and UV-vis
   b. Resonance methods including NMR and EPR, magnetic spectroscopy

10.) Coordination chemistry I
   a. Nomenclature, isomerism (IC 9.1 to 9.3.4)
   b. Chelating ligands, coordination numbers and geometries (IC rest of Ch. 9)

11.) Transition metal complexes
   a. Crystal and ligand field theories, the spectrochemical series (IC 10.2 to 10.3.3,
       MSGT 7.1)
   b. 4- and 6-coordinate complexes, Jahn-Teller effects (IC rest of Ch. 10, MSGT 7.2)
   c. The MO approach to TM complexes (MSGT 7.3)
   d. Term symbols, splitting and (MSGT 7.5, IC 11.2)
   e. The electronic spectra of d-metal complexes Tanabe-Sugano diagrams (MSGT
       7.6, IC Ch. 11.3)

12.) Coordination chemistry II
   a. Reaction mechanism: Substitutions (IC 12.1 to 12.4.3, and 12.6 to 12.7)
   b. Reaction mechanisms: Electron transfer, oxidation-reduction (IC 12.8)

13.) Organometallic chemistry
   a. 18-electron rule and carbonyl complexes (IC 13.1 to 13.4.1)
   b. Nitrosyl and pi-system complexes (IC 13.4.2 to 13.5.2)

14.) Multiple bonding and inorganic clusters
   a. The isolobal principle, and metal-metal bonding complexes (IC 15.1 to 15.3.1)
   b. Inorganic clusters, rings, and chains (IC 15.4 to 15.4.4)

15.) Materials and solid state chemistry (handouts)
   a. Silicates, zeolites, metal-organic frameworks, and other microporous materials
   b. Magnetic molecules and materials
   c. Nanomaterials

Tentative schedule for problem sets and exams:

Sept. 10: P-set 1 due
Sept. 17: P-set 2 due
Sept. 24: P-set 3 due
Oct. 3: Exam 1
Oct. 15: P-set 4 due
Oct. 22: P-set 5 due
Oct. 29: P-set 6 due
Nov. 7: Exam 2
Nov. 19: P-set 7 due
Dec. 3: P-set 8 due
Dec. 19: Final exam