

The Graduate Center, CUNY
Advanced Inorganic Chemistry (Chem 71000)

Textbook: (Available at Brooklyn College Bookstore)

Inorganic Chemistry, Gary L Miessler and Donald Tarr, 5th Ed, Pearson – Prentice Hall (2013)
Solutions Manual for Inorganic Chemistry (Miessler & Tarr) - Inorganic/organic molecular models

Other recommended books:

-*Inorganic Chemistry*, Catherine E. Housecroft and Alan G. Sharpe, 4th Ed., Pearson – Prentice Hall (2012)

-*Shriver and Atkins Inorganic Chemistry*, 5th Ed., by Atkins Overton, Rourke, Weller, Armstrong, and Hagerman; Freeman (2010) – Note: 6th Edition will be available in January 2014

-*Molecular Symmetry and Group Theory* by Alan Vincent, Wiley, 2nd Ed. (2001)

This is an advanced course and students are expected to do much work on their own. Lectures may not cover all the contents listed below, but students will be expected to know the assigned material. Questions and discussion during the lectures are strongly encouraged. **Reading/writing assignments on original research papers that count toward the grade are recommended to all instructors.**

CONTENT

Unit 0 (Self study; this is basic material that students are expected to know but will not normally be covered in the lectures)

- Revision of basic concepts: *Chapters 1-3 M&T*.
What is inorganic chemistry? Genesis of the elements. Fundamental atomic theory. Quantum numbers and atomic wave functions. Electron configurations of atoms and ions. Periodic trends. Lewis dot diagrams, resonance structures and formal charge. VSEPR theory.

CORE CONTENT

Unit 1 (~5 lectures)

- *Chapter 4 M&T*
Symmetry and group theory: symmetry elements and operations. Point groups. Reducible and irreducible representations of groups. Character Tables. Applications to vibrational spectroscopy. Prediction/interpretation of spectra.

Unit 2 (~5 lectures)

- *Chapter 5 M&T*
Molecular orbitals as linear combinations of atomic orbitals.
Qualitative description of bonding, antibonding and non-bonding interactions.
MO diagrams for homonuclear diatomic molecules for first and second period elements. Orbital mixing. Photoelectron spectroscopy.
MO diagrams for heteronuclear diatomic molecules: CO, HF, LiF. Frontier orbitals
MO diagrams for larger molecules. Symmetry adapted linear combinations (SALCs) of atomic orbitals H-F-H; [F-H-F]; CO₂; H₂O; NH₃; BF₃.
Generalized method for building MO diagrams of larger molecules using tabulated SALCs.
- *Chapter 6. Sections 6.2 and 6.3.*
Frontier orbitals and acid-base behavior. MO interpretation of hydrogen bonding and hard-soft acid-base interactions.

Unit 3 (~5 lectures)

- *Chapter 7 M&T*
The crystalline solid state: cubic, body-centered cubic, and close-packed structures.
Metallic crystals, binary compounds and more complex compounds.
Born-Haber cycles and lattice energy
Molecular orbitals and band structure of solids: valence band and conduction band. Insulators, conductors, and semiconductors. Diodes, the photovoltaic effect and light-emitting diodes.

Quantum dots.

Superconductivity: low T superconducting alloys. Cooper pairs. High T superconductors.

Bonding in ionic crystals and imperfections in solids. Defects: vacancies, non-stoichiometric compounds, solid solutions, and dislocations.

Unit 4 (~ 6 lectures)

- *Chapter 9 M&T*

Coordination chemistry: Nomenclature, isomerism, coordination numbers and geometries.

- *Chapter 10 M&T*

Electronic structure and bonding: From crystal field to ligand field to MO theory. Magnetic susceptibility and magnetic moment. MO diagrams for octahedral complexes, orbital splitting and electron spin. Weak and strong field ligands and the 18 electron rule. Ligand field stabilization energy. MO diagrams for square planar and tetrahedral complexes. The spectrochemical series. Jahn-Teller effects.

- *Chapter 11 M&T*

Electronic spectra: Quantum numbers for multielectron atoms – microstates and electronic terms; spin-orbit coupling. Correlation diagrams and Tanabe-Sugano diagrams. Prediction and interpretation of electronic spectra involving *d-d* transitions. Charge transfer spectra.

- *Chapter 12 M&T*

Reactions and mechanisms

Substitution reactions. Inert and labile compounds. Kinetics and mechanisms of dissociative and associative substitution in octahedral and tetrahedral complexes. Experimental evidence. Stereochemistry. The trans effect.

Redox reactions: inner and outer sphere mechanisms. Basic elements of Marcus' theory.

SPECIAL TOPICS (~5 lectures)

(THESE ARE EXAMPLES AS SPECIAL TOPICS MAY VARY WITH INSTRUCTOR)

- *Chapters 13-14 M&T*

Elements of organometallic chemistry: Ligand types and the 18-electron rule. Synthesis, properties and reactions of selected types of complexes: Metal-carbonyls. Coordinated hydrogen and metal hydrides. Metal-alkene and related complexes. Metal alkyls, carbenes and carbynes. Metallocene and arene complexes. NMR characterization of organometallic compounds.

Reactions of organometallic complexes: association-dissociation; oxidative addition-reductive elimination; attack on coordinated ligands.

Organometallic catalysis: hydrogenation, olefin metathesis, hydroformylation, methanol oxidation, olefin polymerization.

- *Chapter 16 M&T*

Elements of bioinorganic chemistry: Metalloporphyrins. Hemoglobin and myoglobin. Cytochromes, peroxidases and catalases. Chlorophylls. Zinc enzymes.

Inorganic medicinal chemistry: Platinum complexes in cancer treatment. Other medicinal applications of transition metal complexes.