

**CHEM 5310 Advanced Inorganic Chemistry I**  
**Inorganic and Organometallic Reaction Mechanisms**  
**Fall 2016**

Tuesday and Thursday 9:30 – 10:45 AM, CAB 389

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Office Hours: Monday 12:30 – 1:30 PM and Wednesday, 2:00 – 3:00 PM

**Books**

There will be no required textbook for this course. However, several books will be placed on reserve in Chemistry Library. You will be referred to these books for material to supplement the lecture when appropriate.

You will receive references to manuscripts during the course of the semester and are advised to find these papers and carefully read them. Supplementing the lecture and problem sets with literature reading is vital to your comprehension of the material and will greatly enhance your understanding and performance.

**Problem Sets**

Throughout the semester you will be given problem sets. These will be for your benefit and will not count toward your grade. Answer keys will be posted on the course collab site. Check to be sure that the CHEM 5310 collab site is available to you.

**Grading**

Exam I: 30% of grade (likely week of September 26)

Exam II: 30% of grade (likely week of November 7)

Final Exam: 40% of grade (December 13, 2:00 – 5:00 PM)

**Course Outline:** (Note: the order or presentation may be altered)

I. Basics of organometallic chemistry

- Introduction to coordination complexes
- Molecular orbital theory
- Organometallic complexes, the eighteen electron rule, electron counting and oxidation states
- Survey of ligands and metal-ligand  $\pi$ -bonding
- Electronic structure and coordination geometries
- Rotational barriers and bond deformations
- Electronic structure and reactivity
- Agostic bonding and hydrocarbon coordination

II. Tools of the trade

- Kinetics, thermodynamics
- Timescales of physical methods
- Dynamic NMR spectroscopy (brief theory, application toward mechanistic studies)
- Kinetic isotope effects

III. Reactions of organometallic complexes

- Reaction classes
  - Ligand substitution (associative, dissociative,  $I_a$ ,  $I_d$ )
  - Oxidative addition
    - Polar two-step, radical, electron transfer, concerted
  - Reductive elimination
  - Migratory insertion/deinsertion
- Reactions and Seminal Mechanistic Studies (pending available time)
  - Monsanto acetic acid process
  - Hydroformylation (cobalt to rhodium to water to teflon ponytails)
  - C-H activation
  - Olefin metathesis
  - Dinitrogen activation
  - Heck, Suzuki, Stille, Negishi, etc.
  - Catalytic hydrosilation, hydrogenation, and hydrocyanation

### **Books on Reserve in the Chemistry Library**

- 1) *The Organometallic Chemistry of the Transition Metals* by Crabtree
- 2) *Principles and Applications of Organotransition Metal Chemistry* by Collmann, Hegedus, Norton and Finke
- 3) *Chemical Kinetics and Reaction Mechanism* by Espenson
- 4) *Mechanism and Theory of Organic Chemistry* by Lowry and Richardson
- 5) *Concepts and Models of Inorganic Chemistry* by Douglas, McDaniel and Alexander
- 6) *Inorganic Chemistry* by Miessler and Tarr
- 7) *Advanced Organic Chemistry: Part A* by Carey and Sundberg (ELECTRONIC)
- 8) *Basic one and Two-Dimensional NMR Spectroscopy* by Friebolin
- 9) *Modern NMR Spectroscopy* by Sanders and Hunter
- 10) *Orbital Interactions in Chemistry* by Albright, Burdett and Whangbo
- 11) *Metal Ligand Multiple Bonds* by Mayer and Nugent
- 12) *Inorganic and Organometallic Reaction Mechanisms* by J. Atwood
- 13) *Organotransition Metal Chemistry: From Bonding to Catalysis* by J. Hartwig