

# STRUCTURE AND BONDING: CHEM\*2060

Fall 2011

*Last revision Aug 30 2011*

**Course Professor:** Mark Baker: MacN 122: Ext. 58637  
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**Lectures:** MWF MACN 113 11.30 –12.20: start September 9. Note no lecture on October 10 (Thanksgiving). Make up is on Dec 1.

**Tutorial/Problem Session.** Tuesdays 1- 2.20 LA 204 (No class first week.) There may be a class in week 2). In these classes we will look at molecular models, solids do problems and practice exams.

## **Course Evaluation:**

Two in class quizzes: 30% (Held in Tuesday classes: Multiple Choice/ Short answers)

Mid-Term Exam: 30% (30 Multiple Choice Questions)

Final Exam: 40%

**Exams:** Practice Exams will be handed out in class.

## **Exam Schedule:**

Quiz # 1 Sept 27 Room TBA (Week 4): Point groups & symmetry

Mid-Term Exam: Oct 25: (Week 8): All material up to lecture 17

Quiz # 2 Nov. 15 Room TBA (Week 11): Intro to Quantum Chemistry & hybrid orbitals

Final: Dec 9 2.30-4.30: Cumulative.

**Prerequisites:** CHEM-1050, PHYS-1001 and MATH-1210

**Objectives:** This course provides a modern introduction to the shapes and electronic structures of atoms, molecules, polymers and solids. It presents the basic principles regarding chemical structure and bonding. The second half of the course introduces Quantum Chemistry.

**Textbook:** NONE

**Lecture Notes:** Lecture Notes on web. You will be able to download these as pdf's soon when I have uploaded them. Don't use notes from previous years (even if they are mine) because I have revised the notes.

**Office Hours:** Monday morning: 9-11 Also most other times. My door is usually open! Come by yourself or with others. The more the merrier!

**Topics (Lecture Hours): Approximate**

1. **(6 Lectures) Structure and Shape.** Atomic and molecular dimensions. Shapes and structural features of molecules, polymers, surfaces, and solids. Symmetry and shape. Symmetry operations and point group classification.
2. **(6 Lectures) Electrostatic Interactions.** Periodic trends in ionization potentials, electron affinities and electronegativities. Electronic configurations of atoms and ions. Electrostatic interactions between atoms and molecules. Monopoles and dipoles, dispersion forces. Hydrogen bonds and other weak intermolecular interactions. Van der Waals forces.

### *QUIZ*

3. **(6 Lectures) Ionic bonding in molecules and solids.** Madelung effects; estimation and chemical significance of lattice energies. Crystal packing, site symmetry of ions, vacancies. Crystal planes and surface. Introduction to diffraction methods.

### *MID-TERM EXAM*

4. **(8 Lectures) Introduction to quantum concepts in chemistry.** De Broglie wavelength, electron diffraction, the Pauli exclusion principle, Heisenberg uncertainty principle, Schrodinger equation. Detailed treatment of particle in a box in one and three dimensions; Discussion of the energies and wavefunctions for the hydrogen atom. Orbital symmetry.
5. **(6 Lectures) The covalent bond.** Formulation of hybrid orbitals, qualitative and quantitative aspects of valence bond and LCAO molecular orbital models for homo- and heteronuclear diatomic molecules. Elements of frontier orbital theory.

## QUIZ

6. **(4 Lectures) Introduction to the electronic structure of larger systems.** Conjugated organic  $\pi$ -systems, e.g., ethylene, butadiene, benzene. Diels Alder reactions. Frontier orbitals. HOMO-LUMO. Energies and symmetries of  $\pi$ -MO's.

## FINAL EXAM

### **EVALUATION OF PROFESSOR:**

*“As part of the faculty evaluation process in the Department of students are reminded that written comments on the teaching performance of the lecturer may be set to the Chairman, Department of Chemistry at any time. Such letters must be signed.”*

Good books: You can find many books in the library dealing with the ideas that are presented in the lectures. You should try to read from as many sources as possible. Each presentation will be slightly different and it is to a certain extent a matter of personal taste as to which text is the best.

Two Examples:

1. Inorganic Chemistry: D.F. Shriver, P.W. Atkins and C.H. Langford. (W.H. Freeman)
2. Basic Inorganic Chemistry: F.A. Cotton, G. Wilkinson and P.L. Gaus.
3. Chemical Structure and Bonding”: Roger DeKock and Harry B. Gray: University Science Books.

Web Stuff: There are some links given in the notes to good web resources – many others are available and I encourage you to explore them.