CHEM 515 Syllabus – Fall, 2005

I. General Information:

Instructor: Robert K Szilagyi, Assistant Professor
Gaines 223, Phone: 4263, Email: Szilagyi@Montana.EDU
Website: WEBCT – course CHEM51501f05

Lectures: Tue and Thr, 1:30 to 2:50 pm in Gaines 33

Office hours: Mon 3-5 pm (homework discussions) and by appointment

Objectives: The primary objective of this course is to define the basic concepts of structure and bonding in coordination compounds, including atomic theories, valence bond and molecular orbital theories, and to demonstrate the use of these theories in problems of inorganic and organometallic chemistry. A secondary objective is to provide basic knowledge for interpreting spectroscopic features and describing trends employing theoretical models.

Cotton: Chemical Applications of Group Theory (3rd ed.) 1990
(all available at the MSU bookstore)

Exams: Oct 6, Thr form Lectures 1-10
Nov 8, Tue from Lectures 11-18
Nov. 21, Mon presentation abstract due (minimum requirement: title, a paragraph with 3 sentences - what/why/how)
Nov. 28, Mon paper outline due (minimum requirement: title, introduction, methods, analysis, discussion, references)
Dec. 1, Thr final paper due (at least three pages incl. figures/tables)
Dec 7, Wed paper reviews
Dec 8, Thr paper presentations 1:00 to 3:00 pm
Dec 13, Mon comprehensive final exam

Grading: 

midterm exams 40% (20/20%)
final exam 30%
homework 15%
paper 5%

1% format: take the time to prepare it electronically
2% content: scientific insights
1% discussion: your ideas and opinions
1% references: familiarity with other's ideas

paper review 5%
presentation 5%
II. Course Policies and Procedures

There will not be any attendance check prior to the lectures; however, those with better attendance generally score higher on exams. The examinations are based directly on the material from DMA/MT and what is presented in the lectures. The problem sets at the end of each DMA/MT chapter are excellent and the homework will be selected from these problem sets. After turning in the homework assignments, I am available to discuss the solution during office hours.

You must contact me to request a makeup test prior to the exam date if you cannot make the test on the scheduled date. Absence from an exam will result in a grade of zero.

You are responsible for knowing and observing University policies regarding academic dishonesty. See University publication: “Conduct Guidelines and Grievance Procedures: Section 340.00 Academic Honesty.” For additional information please visit www2.montana.edu/policy/student_conduct/ page.

Section 310.00 in the MSU Conduct Guidelines states that students must be prompt and regular in attending classes, well prepared for classes, take exams when scheduled, act in a respectful manner toward other students and the instructor and in a way that does not detract from the learning experience.

III. Course Schedule:

September

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<td>Introduction and Overview</td>
<td>Atomic Structure I</td>
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<td>6 Atomic Structure II</td>
<td>8 Molecular Models I</td>
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<td>27 Molecular Orbitals I</td>
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October

| 4 Molecular Orbitals III | 6 Exam on DMA Ch. 1-4 |
| 11 Coordination Compounds I | 13 Spectra and Bonding I |
| 18 Spectra and Bonding II | 20 Spectra and Bonding III |
| 25 Spectra and Bonding IV | 27 MO of Coordination Compounds |

November

| 1 Organometallic Chemistry I | 3 Organometallic Chemistry II |
| 8 Exam on DMA Ch. 9,10,12,13 | 10 Inorganic Spectroscopy |
| 15 Ground State Methods I | 17 Ground State Methods II |
| 22 Excited State Methods I | 24 Thanksgiving Day – no class |
| 29 Excited State Methods II |

December

| 6 Electronic Structure Calculations | 1 Excited State Methods III |
| 12 Final Exam | 8 Paper presentations |
IV. Course Content:
Lectures 1-2: Atomic structure and the Periodic table
- Bohr model of the atom
- Pauli exclusion principle, quantum numbers
- Spectroscopic terms, vector model, electron configuration
- Wave mechanics, the Schrödinger equation, solution for hydrogen

Lectures 3-4: Molecular Models
- Valence bond theory, Lewis structure, Coordinative bonding
- Resonance structures, hybridization, $\sigma$ and $\pi$ bonding
- Shape of the molecules, qualitative VSEPR model
- Hydrogen bonding and other weak interactions

Lectures 5-7: Symmetry
- Symmetry elements and symmetry operations
- Symmetry point groups
- Character tables, irreducible representations, labeling
- Chemical application of symmetry (vibrations, selection rules)

Lectures 8-10: Molecular Orbitals
- MO theory, LCAO, $\sigma$-, $\pi$- and $\delta$-type orbitals
- Homo and heterodiatomic molecules
- Triatomic molecules – group theoretical treatment
- Cyclic planar molecules

Lectures 11: Coordination Compounds
- Nomenclature of coordination compounds
- Valence bond models, hybridization, orbital occupancy
- Electrostatic bonding and ligand-field theory in octahedral symmetry
- Distortion from octahedral symmetry

Lectures 12-16: Spectra and Bonding
- Ligand field and charge transfer spectra, selection rules
- Splitting in $d^n$ complexes, Orgell and Tanabe-Sugano
- Complexes with lower symmetry than $O_h$
- Molecular orbital picture of bonding in coordination compounds

Lectures 17-18: Organometallic Chemistry: metal-ligand bonding
- Carboxyl complexes, counting rules, IR spectroscopy
- Phosphine, isocyanide, nitrosyl complexes
- Olefin $\pi$-complexes, donation/backdonation
- Single, double, triple metal-carbon bonds

Lectures 19-25: Physical Inorganic Chemistry
- Overview of spectroscopic techniques used in inorganic chemistry
- Magnetization, Mössbauer, EPR, ENDOR, ESEEM
- ABS/CD, Photoelectron, NEXAS and EXAFS
- combination techniques: resonance Raman, MCD, RIXS
- electronic structure calculations
V. Recommended Readings

**Reference Books:**

**Inorganic Textbooks:**

**Organometallics:**

**Bioinorganic:**

**Online References:**
M. Winter, University of Sheffield, U.K. *WebElements* at www.webelements.com