CHMY 515 Syllabus – Fall 2009

I. General Information:
Instructor: Robert K Szilagyi, Associate Professor
Chemistry/Biochemistry Building 253, Phone: 4263,
Email: Szilagyi@Montana.EDU
Research website: computational.chemistry.montana.edu
Course website: eu.montana.edu login with your MSU-ID

Lectures: Mon, Wed, and Fri, noon-1:00 pm in Roberts Hall 102
Office hours: Tue 3-5 pm - homework discussions as needed

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.

Course text: Your undergraduate inorganic chemistry textbook or
Miessler, Tarr (MT): Inorganic Chemistry (3rd ed.) 2003, Wiley, ISBN 978047151094 9; and

Exams: Oct 5, Mon from Lectures 1-13
Nov 4, Wed from Lectures 14-25
Nov 7, Fri review for proficiency
Nov 11, Wed Proficiency Exam (tentative)
Nov. 16, Mon pre-proposals are due (minimum requirement: title, brief intro – what/why/how, and three aims)
Nov. 30, Mon proposals are due (at least three specific aims, max 10 pages incl. figures/tables/references)
Dec. 4, Fri proposal reviews are due
Dec. 7, 9, 11 mock oral examinations during regular class hours
Dec. 16, Wed comprehensive final exam (tentative)

Grading: midterm exams 40% (20/20%)
final exam 30%
homework 15%
proposal 15% (proposal, review, defense)
contribution to online materials extra 5%

grading scheme: A 100-86% (90 A; 86 A-)
B 85-66% (82 B+; 78 B; 74 B-)
C 66% or less (70 C+)
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 in your textbook and those presented in the lectures. The problem sets assigned for your homework are excellent preparations for the midterm exams. After turning in the past week homework assignments by every Monday at noon, I am available to discuss the solutions during office hours.

You must contact me to request a make up test prior to the exam date if you cannot make the test on the scheduled date. Absence from an exam will result in a score 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:

<table>
<thead>
<tr>
<th>M</th>
<th>W</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>August</td>
<td></td>
<td></td>
</tr>
<tr>
<td>31</td>
<td>Introduction/Overview</td>
<td></td>
</tr>
<tr>
<td>September</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>Labor Day – no class</td>
<td>9</td>
</tr>
<tr>
<td>14</td>
<td>Molecular Models II</td>
<td>16</td>
</tr>
<tr>
<td>21</td>
<td>Symmetry II</td>
<td>23</td>
</tr>
<tr>
<td>28</td>
<td>Molecular Orbitals I</td>
<td>30</td>
</tr>
<tr>
<td>October</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>Exam I</td>
<td>7</td>
</tr>
<tr>
<td>12</td>
<td>Spectra and Bonding I</td>
<td>14</td>
</tr>
<tr>
<td>19</td>
<td>Spectra and Bonding IV</td>
<td>21</td>
</tr>
<tr>
<td>26</td>
<td>MO of coord. comps. III</td>
<td>28</td>
</tr>
<tr>
<td>November</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Organometallic Chemistry III</td>
<td>4</td>
</tr>
<tr>
<td>9</td>
<td>Inorganic Spectroscopy II</td>
<td>11</td>
</tr>
<tr>
<td>16</td>
<td>Ground State Methods II</td>
<td>18</td>
</tr>
<tr>
<td>23</td>
<td>Thanksgiving – no class</td>
<td>25</td>
</tr>
<tr>
<td>30</td>
<td>Excited State Methods III</td>
<td></td>
</tr>
<tr>
<td>December</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>Proposal presentations</td>
<td>9</td>
</tr>
<tr>
<td>16</td>
<td>Final Exam</td>
<td></td>
</tr>
</tbody>
</table>
IV. Course Content:

Lectures 1-3: 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 atoms

Lectures 4-6: Molecular Models
- Valence bond theory, Lewis structure, coordinative/dative bonding
- Resonance structures, hybridization, $\sigma$ and $\pi$ bonding
- Shape of the molecules, qualitative VSEPR model
- Hydrogen bonding and other weak interactions

Lectures 7-10: Symmetry
- Symmetry elements and symmetry operations
- Symmetry point groups
- Character tables, irreducible representations, labeling
- Using 'Molecule' program to "design" symmetrical molecules

Lectures 11-13: Molecular Orbitals
- MO theory, LCAO, $\sigma$-, $\pi$- and $\delta$-type orbitals
- Homo and heterodiatomic molecules
- Triatomic molecules – group theoretical treatment
- (Cyclic planar molecules)

EXAM – I (October 5, Mon noon-2 pm)

Lectures 14-15: 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 16-22: Spectra and Bonding
- Ligand field and charge transfer spectra, selection rules
- Splitting in $d^\pi$ complexes, Orgell and Tanabe-Sugano
- Complexes with lower symmetry than $O_h$
- Molecular orbital picture of bonding in coordination compounds

Lectures 23-25: Organometallic Chemistry: Metal-Ligand Bonding
- Carbonyl complexes, counting rules, IR spectroscopy
- Phosphine, isocyanide, nitrosyl complexes
- Olefin $\pi$-complexes, donation/backdonation
- Single, double, triple metal-carbon bonds

EXAM – II (November 4, Wed noon-2 pm);
ACS proficiency exam (November 11, Wed 3-5 pm)

Lectures 26-34: 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 (all available at the MSU Library)

Reference Books:

Inorganic Textbooks:

Organometallics:

Bioinorganic:

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