Drexel University University Molecular Symmetry and Group Theory CHEM 420 Winter 2014 Syllabus

Instructor: Dr. Molly A. O'Connor Office: Stratton 410
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CLASS SCHEDULE

Lecture: T Th 2:00 – 3:20 pm Pearl 302

Office Hours: T 10:30 am – 12:30 pm Stratton 410

W 1:00 – 3:00 pm Stratton 410

Also available by appointment

COURSE OBJECTIVES

 To understand how structure and bonding influence the physical properties and reactivity of inorganic molecules.

- To be able to use crystal field theory to understand the electronic and magnetic properties of transition metal complexes.
- To be able to use symmetry to predict molecular orbital diagrams and explain electronic spectra.
- To gain an appreciation for how inorganic chemistry influences your everyday life.

Note – CHEM 421 is the pre-requisite for CHEM 420. Junior chemistry majors follow CHEM 421 with CHEM 420 in the winter term (either the same year or the next year), with CHEM 422 and CHEM 425 taken in the spring of your Senior year.

COURSE MATERIALS

Required:

- Vincent, A. *Molecular Symmetry & Group Theory 2nd ed.*; Wiley, 2001.
 - o available as a 2-hour loan *via* Hagerty Reserves
- Any molecular model kit that can build linear, trigonal planar, tetrahedral, trigonal bipyramid, and octahedral structures

Other Useful Texts:

- Housecroft, C. E.; Sharpe, A. G. *Inorganic Chemistry 4th ed.*; Pearson, 2012. ISBN: 978-0-273-74275-3.
 - o 3rd edition available in the library; in the process of acquiring the newest edition
- Atkins, et al. *Shriver & Atkins Inorganic Chemistry 5th ed.*; Freeman, 2010.
 - o available as a 4-hour loan via Hagerty Reserves

- Lawrence, G. A. *Introduction to Coordination Chemistry*, Wiley, 2010.
 - o available as a hardcopy and as an electronic resource via Hagerty Library
- Miessler, G. L.; Tarr, D. A. *Inorganic Chemistry 3rd ed.*; Pearson, 2004.
 - o available as an overnight loan via Hagerty Reserves

Web: The "Drexel Learn" course website will be used extensively throughout the course. Lecture notes, course announcements, homework assignments and solutions, and exam information will be regularly posted. Emails will also be sent to your Drexel email account. Students are responsible for checking the course website and email on a regular basis.

COURSE EXPECTATIONS

Lecture: Lecture will primarily be conducted through PowerPoint lectures as well as through worked examples on the board, in-class demonstrations, and in-class activities. The PowerPoint lectures will be posted on the course website, typically immediately following class. Though lecture is the major portion of the course, students must also refer to outside material to gain a full understanding of the curriculum. Relevant readings for most of the topics can be found in any inorganic textbook. The Vincent text is very useful for the MSGT portion of the course.

Attendance: Although an attendance grade will not be given in this course, you are expected to attend all lectures. If you do miss class, be sure to go over the corresponding PowerPoint slides and consult a fellow classmate for any additional notes given in class. You are also expected to arrive on time and remain to the end of class. Arriving late or leaving early puts the student at a disadvantage as well as interrupts the rest of the class. If you must arrive late or leave early, please notify me beforehand.

Homework Problem Sets: Five homework sets will be assigned throughout the term. Regular work on problems is <u>ESSENTIAL</u> to your mastery of the topics presented in CHEM 420. You are encouraged to discuss these problems with me at our mutual convenience, as well as with your classmates, though final work turned in for grading must be your own. Due–dates for homework assignments are included in the syllabus. Assignments are typically due by 11:59 pm on the date indicated. You may submit assignments electronically to the following email address: maoconnor83@gmail.com. Late homework assignments will result in a deduction of 10% per day. Homework will not be accepted once assignments have been returned, or answer keys have been posted. Assignments will be posted on the course website at least one week prior to the due date. Problem sets will be graded mostly on effort, but the instructor reserves the right to choose a few questions at random for grading based on performance. Answer keys will be posted on the course website once the assignment has been returned. Be sure to go over the key so that you learn from your mistakes prior to an exam!

Exams: There will be two one-hour exams during the semester and a 2-hour comprehensive final exam. The exam dates for the in-class exams can be found on the class schedule at the end of the syllabus. The date, time, and place of the final exam will be announced later in the term so do not make any travel arrangements until you know your final exam schedule. All exams, including the final, will be closed book. If you miss an in-class exam, a make-up exam will be given at the end of the term (date, time, and place of the make-up exam are TBA). You do not need an excuse to take the make-up if you miss an in-class exam, but you *MUST* attend the make-up or receive a score of zero. You may make-up only one exam, and only because of an absence. NO MAKE-UP EXAMS WILL BE GIVEN FOR THE FINAL EXAM!

Please let me know as soon as possible if you require extended time for exams or have any additional needs. Proper paperwork is required and must be filled out through the Office of Disability Resources. Students with disabilities should see material under the "health and disability services" tab at the following link: http://drexel.edu/studentaffairs/community_standards/studentHandbook/

Electronic Devices: Students may use computers, laptops, and electronic tablets to follow along with the lecture notes. The use of computers, laptops, and electronic tablets for *any other purposes*, as well as the use of cell phones, iPods, mp3 players etc., will be *strictly prohibited* during class! If students are unable to abide by these rules, all electronic devices will be prohibited!

GRADING

Tentative grade cutoffs are shown below. The instructor reserves the right to lower some or all of the grade cutoffs.

| Final Letter Grade | A | A- | B+ | В | В- | C+ | С | C- | D+ | D | F |
|--------------------------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------------|
| % | 100-93 | 92-90 | 89-87 | 86-83 | 82-80 | 79-77 | 76-73 | 72-70 | 69-67 | 66-65 | Below 65 |

The grading rubric for the course is as follows:

| Homework | 10% | | |
|----------------|-----|--|--|
| In-class Exams | 50% | | |
| Final Exam | 40% | | |

Academic Integrity: Discussion of lecture material and homework assignments among class members is encouraged, but all final work turned in for grading must be your own, unless otherwise explicitly stated. Academic dishonesty in any form (plagiarism, cheating, copying homework, or use of unauthorized answer keys) will not be tolerated and will result in an **AUTOMATIC ZERO** on the given assignment. Subsequent incidents of academic dishonesty will result in automatic failure of the course. For more information, see material in "academic dishonesty" under the "academic policies" tab at the following link:

http://drexel.edu/studentaffairs/community_standards/studentHandbook/

Course Withdrawal: If you are registered and wish to drop or withdraw from this course, see the following link: http://www.drexel.edu/provost/policies/course_drop.asp. Also, please note the following important dates from the University registrar:

- Last day to drop/add with Academic Advisor assistance: Friday January 17th
- Last day to drop/add via DrexelOne (by 11:00 pm): Sunday January 19th
- Last day for withdrawal: Friday February 21st

TENTATIVE SCHEDULE

The instructor reserves the right to change the schedule of topics, readings, homework assignments, etc., if necessary. Appropriate advance notice will be given by in-class announcement and on the course website. The dates of in-class exams and the final exam will not change.

| Week | Lecture Dates | Lecture Topics | Notes |
|------|-------------------|--|------------------|
| 1 | T 1/7 Th 1/9 | X-ray diffraction review Bond Valence Sum Theory Transition metal ion electron configuration review | |
| 2 | T 1/14 Th 1/16 | Symmetry elements and groups: combination, matrix usage, and characters | HW 1 due Th 1/16 |
| 3 | T 1/21 Th 1/23 | Symmetry elements and groups: combination, matrix usage, and characters continued Reducible and irreducible representations | |
| 4 | T 1/28 Th 1/30 | Reducible and irreducible representations continued Character tables Mullikan Notation | HW 2 due Th 1/30 |
| 5 | T 2/4 Th 2/6 | Character tables and Mullikan Notation continued Exam 1 Review | Exam 1 Th 2/6 |
| 6 | T 2/11 Th 2/13 | Crystal Field Theory O_h fields, spectrochemical series, Jorgensen's f & g values | HW 3 due Th 2/13 |
| 7 | T 2/18 Th 2/20 | • Magnetism • CFS other than O_h : T_d fields, 4d and 5d ions, planer/ D_{4h} symmetry, Jahn-Teller distortion | |
| 8 | T 2/25 Th 2/27 | Symmetry approach to atomic orbitals and molecular orbitals MO theory for transition metal complexes | HW 4 due Th 2/27 |
| 9 | T 3/4 Th 3/6 | Electronic spectra of transition metal complexes introduction Exam 2 Review | Exam 2 Th 3/6 |
| 10 | T 3/11 Th 3/13 | • More electronic spectra including: d-d transitions, ligand π to π^* transitions, LMCT, MLCT, selection rules, Tanabe and Sugano diagrams • Final Exam Review | HW 5 due T 3/11 |
| 11 | | FINAL EXAM: Date, Time, and location TBA | |