UNIVERSITY OF MANITOBA

CHEM 3580: Methods in Physical Organic Chemistry

Course Outline for Winter 2014

Course Instructor and Laboratory Supervisor: Dr. Horace Luong
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Lecture
Lectures are held in room 539 Parker on Monday, Wednesday and Friday 11:30 am-12:20 pm.

Prerequisite:
The prerequisite for this course is CHEM 2220 with a grade of C or better. Students must also have taken or be taking CHEM 2290.

Course Content:
This course will explore how organic chemistry experiments are designed and used to understand physical aspects such as rates, orders, equilibria constants of organic reactions. We will be looking at molecular structure, pericyclic reactions, kinetics and catalysis. This course will cover modern developments in supramolecular chemistry which demonstrates many of topics covered in this course.

Textbook:
"Modern Physical Organic Chemistry" by E. V. Anslyn and D.A. Dougherty (University Science Books) is required.
Textbook solutions manual is optional

Evaluation
The evaluation for CHEM 3580 is as follows (100% total):

Laboratory Work	25%
Assignment (3)	15%
In-Class Presentation	15%
Final Examination	45%

Letter grade division:

≥ 90.0%	A+	67.0 – 73.9%	B	40.0 – 49.9%	D
80.0 – 89.9%	A	60.0 – 66.9%	C+	<40.0%	F
74 – 79.9%	B+	50.0 – 59.9%	C		

Assignment
Three assignments will be given, each worth 5% of your course grade. Below is a schedule of when the assignment will be given and their due dates. The work submitted must be of an individual effort, although students can work with others to deduce their answers.

Assignment	Released	Due Date (at the start of class)
1	Monday January 20, 2014	Monday February 3, 2014
2	Monday February 10, 2014	Monday February 24, 2014
3	Monday February 24, 2014	Monday March 10, 2014

Final Examination
The final examination for this course will be cumulative; you are responsible for everything covered and mentioned in the course syllabus. The final examination will be schedule by the Registrar's Office for April during the final exam period. If the final exam is missed due to medical or other compassionate reasons, then deferrals can only be issued by the student's home faculty.

Review of Final Exam
The Faculty of Science has established a policy to permit students the opportunity to review their final exam script prior to the end of the Grade Appeal Period. The Department of Chemistry has developed a procedure which requires that students complete an application form and pay a fee ($5.00) prior to the review of their final exam script. The Application Form can be obtained from the Department of Chemistry General Office (360 Parker).

Laboratory Program

The CHEM 3580 laboratory is in room 562 Parker Building and occur on Friday afternoons 2:30-5:30 pm. The TA for the laboratory is Mr.Ronald Domalaon (e-mail: umdomala@myumanitoba.ca).
The laboratory schedule is as follows:

Experiment	Date	Report Due Date
1 Week 1 NMR Training	January 17	By February 7, 2014, 2:30 pm
1 Week 2	January 24	
2 Week 1	January 31	By February 28, 2014, 2:30 pm
2 Week 2	February 7	
3	February 14	By March 7, 2014, 2:30 pm
4	February 28	By March 14, 2014, 2:30 pm
5 Week 1	March 7	By March 21, 2014, 2:30 pm
5 Week 2	March 14	
6 Week 1	March 21	By April 4, 2014, 2:30 pm
6 Week 2	March 28	
Lab Notebook		By April 4, 2014, 2:30 pm
Total		

Reports are to be handed to Ronald directly.

The laboratory portion of the grades is worth 25% and a minimum mark of 15/25 is required to pass the laboratory.

Students will also require a laboratory notebook. The laboratory notebook is bound and hardcover. If you have from a different course, you can also use it for this course.

Notebook formatting (adopted from CHEM 3390 laboratory program)

- Number all pages and they must be intact (do not tear pages out)!
- Reserve the first few pages for the table of contents
- Cross errors out with a single line.
- Record observations, yields and melting points.

Basic Components of the Lab Notebook:
Prior to the Lab:

- Date of experiment
- Title
- Reaction scheme (Do not use molecular formulae, but draw out the structures or reactants and products)
- Any literature references
- Table of properties of reagents and product(s) (reference literature sources). Can continue use of CHEM 2220 table formatting.
- Calculations (limiting reagents, masses, and volumes of reagents to use and expected yields) should be performed and recorded in lab book prior to performing the lab. These calculations are to give you a rough idea of what to expect, but record actual amounts used during the lab.

During the Lab:

- Details of procedure actually used in sufficient detail to be exactly reproduced from the lab notebook only
- Unusual equipment used
- Amounts of reagents in appropriate units (mass or volume and moles)
- Sequence of experimental operations
- Method of work-up and isolation/purification
- Colour and temperature changes

After the lab:

- Characteristics of product(s) (m.p., colour)
- Analytical and spectral data tabulated. See additional notes on the organization of the lab notebook in the lab manual

Formal Lab Write-Up:

- Introduction
  - Introduction to and purpose of the experiment
  - Reaction scheme
  - Relevant background and literature
- Experimental
  - Detailed description of what was actually done in the lab
  - Quantities of all reagents (stoichiometry, etc.).
  - Purpose of all reagents
    - Discussion Mechanism of the reaction (if relevant)
  - Answers to questions posed in the experiment
  - Discuss the significance of the experiment, observations and results
  - Assignment of spectra where necessary. Brief description of the assignments of the signals of your product. Please include a table of ^{1}H and ^{13}C signals (chemical shifts in ppm and multiplicity).
  - Outside sources of information to support the discussion are welcome and encouraged, but must be properly referenced as footnotes or endnotes.
- Conclusion
- General quality of report
  - Includes organization, layout, grammar (usually for scientific writing a third person past tense should be used).
  - Scheme and mechanism are not the same thing. A scheme simply shows reactants, reagents, conditions and product. Normally intermediates are not indicated.

General Notes on the Write-Up

The lab report must clearly demonstrate that you understood the purpose and results of your experiment. It is important to be concise in your discussion. Going "above and beyond" in the sophistication in your discussion will be rewarded; however, any inclusion of irrelevant information and unduly long reports will lose marks. If you are unsure of anything, it is better to make an educated guess than to omit information!

The guidelines to the lab report above are just that – guidelines. You may find that different experiments require a different organization or you have a different personal preference. This is fine, just be sure everything is included in the report and that the report is organized in a logical manner.

Laboratory Grade Appeals

No appeals of laboratory grades will be considered after the final examination in the course has been written.

In-Class Presentation

Each student will be required to give a 17 minute presentation followed by a 5 minute question period on a particular supramolecular chemistry system. Students must choose from the following topics:

- Rotaxanes
- Catenanes
- Self-replicating systems (emphasize Julius Rebek's early work)
- Molecular tweezers and clefts
- Synthetic ion channels
- Synthetic ion carriers
- Fluorescent sensors
- Self-Assembly capsules
- Dendrimers
- Chiral Guest Recognition

Students will need to prepare a handout (2-3 pages) to give to the class which summarizes their presentation. The handout will be a study aid because all students in the class will be responsible for the content covered in all of the presentations.

Objective:

Each of the topics listed above can be expanded to cover multiple lectures. The main objectives for this assignment are:

1) Students can work on their presentation skills
2) Students can learn to perform primary source article searching
3) Learn about some of the work going on in the area of supramolecular chemistry

Students should cover the following for their system:

- History of how, when, and who discovered the system
- General synthetic steps to produce the systems
- How is the system characterized (be sure to describe why the particular characterization technique is appropriate)
- Describe the thermodynamics of the system and what allows/how the system works.
- Describe some of the current research (within the past three years) using the system and what makes it so attractive.

Checklist of events:

- January 22 in class - select topic (students should have a look at the list of topics and determine which three or four topics they are interested in prior to Jan 22) and date for presentations.
- Week of March 10 - send PowerPoint slides to Dr.Luong by e-mail and book an appointment to see Dr.Luong (should take about 1 hour) to discuss what will be presented.
- Two days before presentation – send finalized PowerPoint slides or PDF AND handout to Dr.Luong for reproduction and loading onto computer.

Presentations will take place between March 24 – March 31, 2014.

Assessment

Students will be assessed as follows (assessment percentages and criteria are subject to change):

Criteria	**Percentage**
Presentation content (accuracy)	30%
Presentation styles (volume, clarity, flow, presentation aids)	20%
Answer to questions (listening, accuracy)	15%
Handout presentation and content	25%
Peer Assessment (presentation clarity)	10%

Be sure to reference your materials used!

Sources of information

Students should initially consult the course textbook for information on their system (if available). There is an Encyclopedia of Supramolecular Chemistry in the reference section at the Science library which will also be of some help.

Cheating and Plagiarism:

The copying of another student's laboratory reports, assignments or examinations is plagiarism. Plagiarism and other forms of cheating are prohibited. The full description of plagiarism and the possible penalties associated with it are outlined in the General Calendar. If a student copy parts of another person's work, proper credit must be given. See last page attached and the Faculty of Science website regarding plagiarism (http://umanitoba.ca/faculties/science/undergrad/resources/webdisciplinedocuments.html)

Faculty of Science—Suggested Minimum Penalties for Common Acts of Academic Dishonesty
(Note: Other penalties may apply. Contact the Associate Dean of Science for complete list).

Act of Academic Dishonesty	*Suggested Penalty given by Dept.*	*Suggested Penalty given by Associate Dean of Science*
*unauthorized material used in assignment/quiz/test/examination (first offence)	grade of zero on assignment/quiz/ test/examination	
*unauthorized material used in assignment/quiz/test/examination (first offence with clear intent; second or subsequent offence)	**F-CW plus suspension from all departmental courses for a minimum of one full year	Suspension from all Science courses for a minimum one full year
copying in laboratory report/assignment/quiz/test/examination (first offence)	grade of zero on laboratory report/ assignment/quiz/test/examination	
copying in laboratory report/ assignment/quiz/test/examination (first offence with clear intent; second or subsequent offence)	F-CW plus suspension from all departmental courses for a minimum of one full year	Suspension from all Science courses for a minimum one full year
plagiarism on assignment/ project/laboratory report (first offence)	grade of zero on assignment/project/ laboratory report/	
plagiarism on assignment/project/ laboratory report (first offence with clear intent; second or subsequent offence)	F-CW plus suspension from all departmental courses for a minimum of one full year	Suspension from all Science courses for a minimum one full year
inappropriate communication during a quiz/test/examination (first offence)	grade of zero on quiz/test/examination	
inappropriate communication during a quiz/test/examination (first offence with clear intent;second or subsequent offence)	F-CW plus suspension from all departmental courses for a minimum of one full year	Suspension from all Science courses for a minimum one full year
personation on quiz/test/ examination	F-CW plus suspension from all departmental courses for a minimum of one full year	Suspension from all Science courses for a minimum one full year

Also includes possession of unauthorized aid (e.g. cell phone), regardless of whether or not it was actually used. It is essential that instructors define clearly (on their course outline ROASS sheets) which aids are permitted in quizzes, tests, examinations, with all other items being explicitly declared as being unauthorized materials.

****F-CW stands for Failing grade due to Compulsory Withdrawal from the course for Academic Dishonesty reasons.***

Note: Non-Science students found guilty of academic dishonesty in Science courses may also be given additional penalties by their Registration Faculty (e.g. an Engineering student taking a Mathematics course may be receive penalties from the Department of Mathematics, Associate Dean of Science plus Dean of Engineering).

Course content of CHEM 3580

All of the chapters/sections associated with the topics listed below are from Modern Physical Organic Chemistry (based on 37 classes).

1. Molecular structure and thermodynamics (4 classes) (Chapter 1.1-1.4)
    a. Molecular orbital theory and orbital mixing
        i. Types and structures of reactive intermediates
        ii. Carbocations, carbanions, radicals, carbenes/carbenoids
2. Strain and stability (5 classes) (Chapter 2.1-2.5, omit Bredt's Rule)
    a. Thermochemistry of stable molecules
    b. Thermochemistry of reactive intermediates
3. Reactions and kinetics (10 classes) (Chapter 7.1-7.6, 8.1-8.3,8.8)
        i. Transition state theory (Arrhenius, Eyring)
    b. Kinetic/thermodynamic control
    c. Kinetic experiments
        i. Kinetic isotope effect and labelling experiments
        ii. Crossover experiments
        iii. Fast kinetic techniques
        iv. Steady state kinetics
    d. Hammett plots
    e. Intermediates:
        i. The detection of intermediates
        ii. Trapping experiments
        iii. Reactions of intermediates
        iv. Rearrangement reactions
4. Solvent and solution properties (4 classes) (Chapter 3.1-3.2)
    a. Solvent scales
        i. Dielectric constants
        ii. Heat of vaporization
        iii. Surface tension and wetting
    b. Solubility
5. Acid and base catalysis (4 lectures) (Chapter 9.1, Supplement)
    a. Specific acid and base catalysis
    b. General acid and base catalysis
    c. Ester hydrolysis (A1, A2, B1, B2 reaction mechanisms)
6. Molecular recognition and supramolecular chemistry (5 lectures) (Chapter 4.1-4.3)
    a. Binding forces (Ion pairing, electrostatic interactions with dipoles, hydrogen bonding, pi effects, induced-dipole interactions, hydrophobic effect)
    b. Topics as covered in the student presentations
7. Pericyclic Reactions (4 lectures) (Chapter 15.1-15.2.1, 15.2.3-15.4, Supplement)
    a. Electrocyclic reactions
        i. Woodward-Hoffmann rules
        ii. Frontier-orbital theory
        iii. Correlation diagrams
    b. Thermal cycloaddition reactions (secondary orbital effects, photochemical cycloaddition reactions)

Suggested Problems from the Course Textbook:
To determine if you have grasped the material covered in the textbook, I would recommend having a look at these questions at the end of the chapters.
Chapter 1: 4,5,9,10,13,17,18,19,21,22,23,24,25,28,30,31
Chapter 2: 3,5,6,9,10,11,15,16,18,20,26,33,41,43
Chapter 3: 1,2,3,4,9,12,13,18,22,25
Chapter 4: 1,2,3,4,9,10,15,16,17,18,19,
Chapter 7: 2,3,4,5,6,7,10,11,13,15,16,18,22
Chapter 8: 1,2,9,11,12,15,18,19,20,21,22,24,27
Chapter 15: 4,5,6,7,10,12,15,23,25,28,32,33