

Syllabus

Chem 395/425 Special Topics in Organic Chemistry (Fall 2019) "Computational Organometallic Chemistry"

COURSE INFORMATION

Course Instructor

Instructor: Prof. Hee Yeon Cho
Office: Flanner Hall 209
Email: hcho6@luc.edu
Group Website: <http://www.chogroup.org>

Course Schedule

Lecture: Tu/Th 4:15–5:30 PM in Flanner Hall 105

Office Hours: Th 5:30–6:30 PM in Flanner Hall 209

To schedule an alternative appointment, please email me.

Email

You must use your Loyola email address for all communication during this course. Emails from outside sources are often blocked automatically.

Course Materials and Website

Textbooks (*Recommended*):

- Principles and Applications of Organotransition Metal Chemistry
By James P. Collman, Louis S. Hegedus, Jack R. Norton, and Richard G. Finke
ISBN-13: 978-0935702514
- Organotransition Metal Chemistry
By John F. Hartwig
ISBN-13: 978-1891389535
- Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics
By Errol G. Lewars
ISBN-13: 978-3319809151

Course Website: sakai.luc.edu

GRADING POLICY

Course Grade

(1)	2	Homework Grades (100 points each, 200 points)	200	20%
(2)	2	Midterm Exams (200 points each, 400 points)	400	40%
(3)	1	Final Exam (400 points)	400	40%
Total			1000	100%

(1) Homework Problem Sets (200 points, 20%)

There are **two (2)** homework problem sets given during the semester. Each problem set will be worth 100 points. Late submissions will get point deductions.

(2) Midterm Exams (400 points, 40%)

There are **two (2)** midterm exams on 10/3/19 (Thursday) and 11/21/19 (Thursday). The midterm exams cover lecture topics and will be held during the lecture. There are **NO MAKEUP midterm exams**.

(3) Final Exam (400 points, 40%)

The final exam will take place on **Tuesday, December 10 at 4:15–6:15 PM in Flanner Hall 105**. *The final exam is **CUMULATIVE***. All topics discussed during lecture over the semester will be on the final. There is **NO MAKEUP final exam**.

Final Grades

A guideline for grades is shown below. At minimum, you will receive the grade indicated. However, if the class average is below 75% at the end of the semester (i.e. the class average of total point is below 750), there will be a modified grading system. Each exam will not be curved.

A = 94–100%	C+ = 75–77%
A– = 89–93%	C = 66–74%
B+ = 86–88%	C– = 63–65%
B = 81–85%	D = 51–62%
B– = 78–80%	F = 0–50%

Lecture and Homework

The class lectures will be the *most critical source* of information for this course. If you miss a lecture, please find notes from another student in class. The homework problems will reiterate important points made during the lectures and will be similar to exam questions.

Class Etiquette

Come to class on time.

No talking

No electronic devices, but you can use your laptop or tablet for note taking.

Students with multiple violations of classroom etiquette will be subject to point deductions throughout the semester.

COURSE TOPICS & OBJECTIVES**Course Topics**

- I. Introduction & History
 - History of Organometallic Chemistry
- II. Fundamentals of Structure and Bonding
 - Oxidation State & 18 Electron Rule
 - Crystal Field Theory & Ligand Field Theory
 - Types of Ligands
- III. Mechanisms
 - Examples of Organometallic Reactions
- IV. Computational Chemistry
 - Potential Energy Surface
 - Molecular Mechanics
 - Quantum Mechanics in Computational Chemistry
 - Ab initio Calculations
 - Semiempirical Calculations
 - Density Functional Calculations

Course Description and Outcomes

The main objective of this course is to build a fundamental understanding of how organometallic reactions proceed and how computational chemistry can be applied to comprehend the processes. Various types of organometallic reactions will be reviewed in this course, and the fundamentals of computational chemistry will be presented. This foundation of knowledge will allow students to attack new problems in organometallic chemistry that they are faced with as they progress as scientists. This will be achieved by taking an in-depth mechanistic analysis of several organometallic reactions.

COURSE POLICY

Academic Integrity

All students in this course are expected to have read and to abide by the demanding standard of personal honesty, drafted by the College of Arts & Sciences. Anything that you submit as part of your grade in this course (homework, exam, etc.) must represent your own work. Any students caught cheating will, at the very minimum, receive a grade of “zero” for the item that was submitted. If the cheating occurred during a course exam, the incident will be reported to the Chemistry Department Chair and the Office of the CAS Dean. Depending on the seriousness of the incident, additional sanctions may be imposed.

Dropping and Withdrawal

Be aware of the following dates in the semester:

September 3 (Tuesday): Last day to withdraw without a “W” grade

September 8 (Sunday): Last day to withdraw with a 100% Bursar credit

September 22 (Sunday): Last day to withdraw with a 50% Bursar credit

September 29 (Sunday): Last day to withdraw with a 20% Bursar credit

November 1 (Friday): Last day to withdraw with a “W” grade, thereafter a “WF” will be assigned

Course Repeat Rule

Effective with Fall 2017, students are allowed only three attempts to pass Chemistry courses with a C– or better grade. The three attempts include withdrawals (W). After the second attempt, the student must secure approval for a third attempt. Students must come to the Chemistry Department, fill out a permission to register form or print it from the Chemistry Department website: <http://www.luc.edu/chemistry/forms/> and obtain a signature from the Undergraduate Program Director, Assistant Chairperson, or Chairperson in Chemistry. Then, a copy of this form is taken to your Academic Advisor in Sullivan to secure final permission for the attempt.

Disabilities

Students with a university-documented disability should contact me immediately. If your disability requires that quizzes and exams be taken outside of the scheduled time or place, please consult: www.luc.edu/sswd/. Services for Students with Disabilities (SSWD) serves students with disabilities by creating and fostering an accessible learning environment. To accommodate your special requests, I need to receive an official letter from the SSWD center at least a week before the exam date.

Course/Instructor Evaluation – IDEA

Loyola has the IDEA program for instructor and course evaluations. At the end of the semester, you will complete an online evaluation of this course based on criteria set by IDEA and by the instructor. For this course, the main objectives are as follows:

- 1) Gaining factual knowledge (terminology, classifications, methods, trends)
- 2) Learning fundamental principles, generalizations, or theories
- 3) Gaining a broader understanding and appreciation of intellectual/cultural activity

Keep these objectives in mind throughout the course.

CHANGES TO SYLLABUS

There may be changes to the syllabus during the semester. ***You are responsible for all syllabus changes made in class whether or not you attend.***

FALL 2019, CHEM 395/425 Calendar

*** NO MAKE-UP EXAMS (midterm or final) will be given. Plan accordingly.

Week	Monday	Tuesday	Wednesday	Thursday	Friday
1	8/26	8/27 Lecture 1	8/28	8/29 Lecture 2	8/30
2	9/2 Labor Day	9/3 Lecture 3 Last day to drop without "W"	9/4	9/5 Lecture 4	9/6
3	9/9	9/10 Lecture 5	9/11	9/12 Lecture 6	9/13
4	9/16	9/17 Lecture 7	9/18	9/19 Lecture 8	9/20
5	9/23	9/24 Lecture 9	9/25	9/26 Lecture 10	9/27
6	9/30	10/1 Lecture 11	10/2	10/3 MIDTERM 1	10/4
7	10/7 Fall Break	10/8 Fall Break	10/9	10/10 Lecture 12	10/11
8	10/14	10/15 Lecture 13	10/16	10/17 Lecture 14	10/18
9	10/21	10/22 Lecture 15	10/23	10/24 Lecture 16	10/25
10	10/28	10/29 Lecture 17	10/30	10/31 Lecture 18	11/1 Last day to drop without "WF"
11	11/4	11/5 Lecture 19	11/6	11/7 Lecture 20	11/8
12	11/11	11/12 Lecture 21	11/13	11/14 Lecture 22	11/15
13	11/18	11/19 Lecture 23	11/20	11/21 MIDTERM 2	11/22
14	11/25	11/26 Lecture 24	11/27 Thanksgiving	11/28 Thanksgiving	11/29 Thanksgiving
15	12/2	12/3 Lecture 25	12/4	12/5 Lecture 26	12/6 Last Day of Classes!
16	12/9 Final Exams Start	12/10 4:15-6:15 PM FINAL EXAM	12/11	12/12	12/13