Course Syllabus – CHEM 460

Course Information

Course Number: CHEM 460 FA20
Course Name: Physical Organic Chemistry - Bonding and Reactivity
Term: FA 2020
Start Date: 09/08/2020
End Date: 12/11/2020
Credits: 3.0

Meeting Days / Times

Tuesdays and Thursdays, 11:00am-12:30pm PT / 2:00-3:30pm ET
(See Calendar in Canvas for the most up-to-date schedule.)

Location

Online via Zoom

Course Managers

Role	Last Name	First Name	Email Address
Instructor	Houk	K.N. (Ken)	houk@chem.ucla.edu
Instructor	Rebek	Julius	jrebek@scripps.edu
Instructor	Shenvi	Ryan	rshenvi@scripps.edu
TA	Holcomb	Matt	mattholc@scripps.edu

Course Description

The course covers selected special topics pertinent to current research in physical organic chemistry with an emphasis on bonding and reactivity. Topics include molecular structure and thermodynamics, intermolecular forces, reactivity and mechanisms, stereochemistry and electronic structure. Lectures are accompanied by examples from the current literature as well as case studies significant to the historical development of the field. The course is a useful companion to specialized classes in chemical synthesis, organometallic chemistry, and bio-organic chemistry.

Program Learning Outcomes

By the end of the program, students will have accomplished these objectives:
PLO1: Critique peer-reviewed publications
PLO2: Understand approaches and methodologies needed for complex scientific questions
PLO3: Knowledgeable of a wide array of technical research skills used in drug discovery
PLO4: Possess strong communication skills

Course Learning Outcomes

Upon completion of this course students will be able to:
CLO1: Understand the detailed structure of a molecule.
CLO2: Identify a molecule's hot spots with respect to reactivity (factors include sites of acidity, electronegativity, polarizability, atomic and molecular orbital character and strain).
CLO3: Evaluate the contribution of these factors to a molecule's energetics, noncovalent interactions and reaction mechanisms.

Background Preparation (Prerequisites)

Satisfactory completion of an undergraduate course in organic chemistry is required, but previous exposure to physical organic chemistry is not.

Course Materials

Required: Anslyn & Dougherty (2005). *Modern physical organic chemistry*. ISBN: 978-1891389313.
Required: Vogel & Houk (2019). *Organic chemistry: Theory, reactivity, and mechanisms in modern synthesis*. ISBN: 978-3527345328.

Attendance Statement

Students are expected to attend all classes. Students who are unable to attend class must seek permission for an excused absence from the course director or teaching assistant. Unapproved absences or late attendance for three or more classes may result in a lower grade or an "incomplete" for the course. If a student has to miss a class, he or she should arrange to get notes from a fellow student and is strongly encouraged to meet with the teaching assistant to obtain the missed material.

Scientific and Professional Ethics

The work you do in this course must be your own. Feel free to build on, react to, criticize, and analyze the ideas of others but, when you do, make it known whose ideas you are working with. You must explicitly acknowledge when your work builds on someone else's ideas, including ideas of classmates, professors, and authors you read. If you ever have questions

about drawing the line between others' work and your own, ask the course professor who will give you clear guidance. Exams must be completed independently. Any collaboration on answers to exams, unless expressly permitted, may result in an automatic failing grade and possible expulsion from the Graduate Program.

Technology Requirements and Support

For issues related to Canvas, please contact the Graduate Office by email at: gradprgm@scripps.edu or by phone at: 858-784-8469.

Course Grading

Grading is in accordance with the academic policies of the Skaggs Graduate School. The breakdown of grading is as follows:

- Each of the three exams constitutes one third of the final grade.

Letter Grade	Percent	GPA	Description
A	93-100	4.00	Outstanding achievement. Student performance demonstrates full command of the course subject matter and evinces a high level of originality and/or creativity that far surpasses course expectations.
A-	90-92	3.67	Excellent achievement. Student performance demonstrates thorough knowledge of the course subject matter and exceeds course expectations by completing all requirements in a superior manner.
B+	87-89	3.33	Very good work. Student performance demonstrates above-average comprehension of the course subject matter and exceeds course expectations on all tasks as defined in the course syllabus. There is notable insight and originality.
B	83-86	3.00	Satisfactory work. Student performance meets designated course expectations and demonstrates understanding of the course subject matter at an acceptable level.
B-	80-82	2.67	Marginal work. Student performance demonstrates incomplete understanding of course subject matter. There is limited perception and originality.
C+	77-79	2.33	Unsatisfactory work. Student performance demonstrates incomplete and inadequate understanding of course subject matter. There is severely limited or no perception or originality. Course will not count toward degree.

C	73-76	2.00	Unsatisfactory work. Student performance demonstrates incomplete and inadequate understanding of course subject matter. There is severely limited or no perception or originality. Course will not count toward degree.
P	73-100	0.00	Satisfactory work. Student performance demonstrated complete and adequate understanding of course subject matter. Course will count toward degree.
F	0-72	0.00	Unacceptable work/Failure. Student performance is unacceptably low level of knowledge and understanding of course subject matter. Course will not count toward degree. Student may continue in program only with permission of the Dean.
I		0.00	Incomplete is assigned when work is of passing quality but is incomplete for a pre-approved reason. Once an incomplete grade is assigned, it remains on student's permanent record until a grade is awarded.
W		0.00	Withdrew from the course with Dean's permission beyond the second week of the term.

- All courses will be recorded and maintained in the student's permanent academic record; only courses that apply towards the degree will appear on the academic transcript. Non-credit or audited courses will not appear on the transcript.
- 4 core courses taken for a letter grade (pass = B- or higher for a core course)
- 2 elective courses taken pass/fail (pass = A, B, C for an elective)

Because students are encouraged to take electives outside their area of expertise, a "C" letter grade is passing.

Course Schedule:

Date	Details
Mon Sep 7, 2020	Labor Day (No Class)
Tue Sep 8, 2020	Structure and bonding (Rebek)
Thu Sep 10, 2020	Molecular energetics (Rebek)
Fri Sep 11, 2020	Graduate Student Symposium (No Class)
Tue Sep 15, 2020	Conformational analysis (Rebek)
Thu Sep 17, 2020	Electronic effects, strain (Rebek)
Tue Sep 22, 2020	Solutions and non-covalent interactions (Rebek)
Thu Sep 24, 2020	Molecular recognition (Rebek)
Tue Sep 29, 2020	Exam #1
Thu Oct 1, 2020	Acid-based chemistry (Shenvi)
Tue Oct 6, 2020	Carbocations (Shenvi)
Thu Oct 8, 2020	Carbanions (Shenvi)
Tue Oct 13, 2020	Radicals, Radical Ions (Shenvi)
Thu Oct 15, 2020	Exam #2
Tue Oct 20, 2020	Potential and Free Energy Surfaces, Mechanisms (Houk)
Thu Oct 22, 2020	Assignment Thermodynamics, Equilibria, Transition State Theory (Houk)
Tue Oct 27, 2020	KIE, Marcus Theory, Distortion/Interaction Model (Houk)
Thu Oct 29, 2020	Introduction to MO Theory and Computations (Houk)
Tue Nov 3, 2020	Hückel MO Theory and Aromaticity (Houk)
Thu Nov 5, 2020	Excited States and Photochemistry (Houk)
Tue Nov 10, 2020	Frontier MO Theory, Relationship to Substituent Effects (Houk)
Thu Nov 12, 2020	Woodward-Hoffmann Rules and Pericyclic Reactions (Houk)
Tue Nov 17, 2020	Cycloadditions, Huisgen's 1,3-Dipolar Cycloadditions (Houk)
Thu Nov 19, 2020	Sharpless Click Chemistry, Bioorthogonal Cycloadditions and Pericyclases (Houk)
Tue Nov 24, 2020	Exam #3
Thu Nov 26, 2020	Thanksgiving Holiday (No Class)
Fri Nov 27, 2020	Thanksgiving Holiday (No Class)