TEXAS A&M UNIVERSITY

SYLLABUS **CHEM 646**

Course title and number	Physical Organic Chemistry, CHEM 646
Term	Fall 2019
Meeting times and location	MWF 10:20 am – 11:10 am, Room: CHEM 2121

Course Description and Learning Outcomes

Prerequisites: Organic Chemistry I and II or equivalent undergraduate organic chemistry courses.

Physical Organic Chemistry (CHEM646) is a graduate/senior-undergrad level course of advanced organic chemistry. Physical organic chemistry refers to a discipline of organic chemistry that focuses on the relationship between chemical structure and property/reactivity, in particular, applying experimental and theoretical tools of physical chemistry to the study of organic molecules and reactions. Specific focal points of study include the bonding and molecular orbital theory of organic molecules, stability of organic species, transition states, and reaction intermediates, rates of organic reactions, and non-covalent aspects of solvation and intermolecular interactions.

CHEM646 is designed to prepare students for graduate research on broadly defined organic chemistry. This course will provide the students with theoretical and practical frameworks to understand how organic structures impact the properties of organic molecules and the mechanism for organic reactions.

By the end of this course, students should be able to:

1. Gain in-depth understanding of the nature of covalent bonds and non-covalent interactions
2. Use molecule orbital theory to interpret the property and reactivity of organic species.
3. Understand the correlation between the structure and physical/chemical properties of organic molecules, such as stability, acidity, and solubility.
4. Predict the reactivity of organic molecules using thermodynamic and kinetic analyses
5. Probe the mechanism of organic reactions using theoretical and experimental approaches.

Instructor Information

Name	Lei Fang
Telephone	979-845-3186
Email address	fang@chem.tamu.edu
Office hours	TBD after semester begins

Textbook and/or Resource Material

- E. V. Anslyn, D. A. Dougherty, “Modern Physical Organic Chemistry”, 1st Edition, University Science Books.

Course content/grades available online: eCampus.

Grading Policies

Grade assignments for the course will be based upon performance on:

1) In-class exams 3 × 100 pts
2) Group homework assignments 2 × 100 pts
   (One of the above 100 pts will be dropped at the end of semester)
3) Final Examination 200 pts

Total possible pts: 700 – 100 = 600 pts.

Exams: three in-class exams throughout the semester, each worth 100 pts. These exams are

comprehensive, but material covered since the previous test will be emphasized. Tentative dates for the in-class exams: September 23rd; October 26th; November 22nd. These dates are subject to possible change due to unforeseen conflict of schedule. If the exam date has to be rescheduled, you will be notified for at least 1 week in advance.

Group Homework: a number of group homework assignments roughly given biweekly. These assignments will be grouped into two halves, each normalized to 100 pts.

At the end of the semester, your lowest component of either the exams or homework groups (100 total possible pts) will be automatically dropped.

Comprehensive final exam: 200 pts, **8~10 am**, **Dec 10, 2019**.

The final grade will be based on your cumulative performance towards the course total of 600 points. The letter grade is not curved. Helping your peers is encouraged.

Attendance and Make-up Policies

Make-Up examination will be given only for documented excused absences as designed in the official Texas A&M University Student Rules, Section 7.5. If the student is seeking an excused absence, he/she must notify the instructor as soon as possible after the absence, but no later than the end of the second working day after the last date of absence.

For details, see TAMU student rule 7 http://student-rules.tamu.edu/rule07.

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Outline of Course Topics

Entry	Course Content	Text Chapter
1	Bonding and Molecular Orbital Theory	1
	Review of basic concepts; QMOT; Application of QMOT	
2	Strain and Stability	2
	Basic concepts; Energy surface; Bond dissociation energy; Bond stretches and IR spectroscopy; Strains; Electronic effects on stability	
3	Huckel Molecular Orbital Theory of pi-Systems	14.2~14.5
	Schordinger equation and secular equation; Huckel MOT on pi-systems; HMOT of cyclic pi-systems; Application of HMOT	
4	Pericyclic Reactions	15
	Orbital symmetry diagram; Frontier MOT; Cycloaddition and stereochemistry; Pericyclic reaction and sigmatropic reaction	
5	Stereochemistry	6
	Isomerism; Symmetry; Topicity; Center chirality and prochirality; Axial and topological chirality; Polymer tacticity	
6	Solutions and Non-covalent Bonds	3
	Basic concepts; Thermodynamics of solubility and solute behavior; Non-covalent bonds; Molecular dynamics	
7	Supramolecular Chemistry	4
	Thermodynamics of binding; cooperativity; Isotherms and experiments; Molecular recognition; Macrocyclic receptors;	

	Aggregation; Molecular machines	
8	Acid and Base	5
	Basic concepts; pKa in water and in organic solvent; Structure-acidity correlation; Lewis acid-base concept	
9	Energy Surface and Kinetic Analysis	7~8
	Energy surface revisit; Rate and rate constant; Transition state theory; Hammond postulate; Kinetic vs thermodynamic control; Rate laws; Marcus Theory; Experiments for kinetic analysis;	
10	Catalysis	9
	Principles of homogeneous catalysis; Forms of catalysts; Kinetics; Enzymes	
11	Reactions Mechanism	10~11
	Addition; Elimination; Substitution; Isomerization	

* This schedule of activity is subject to change during the semester. The correlated text chapters are assigned arbitrarily at the beginning of the semester and might be updated. Overall, this table only gives you a rough overview of the structure of this course.

Americans with Disabilities Act (ADA)

The Americans with Disabilities Act (ADA) is a federal anti-discrimination statute that provides comprehensive civil rights protection for persons with disabilities. Among other things, this legislation requires that all students with disabilities be guaranteed a learning environment that provides for reasonable accommodation of their disabilities. If you believe you have a disability requiring an accommodation, please contact Disability Services, currently located in the Disability Services building at the Student Services at White Creek complex on west campus or call 979-845-1637. For additional information, visit http://disability.tamu.edu**.**

Academic Integrity

"An Aggie does not lie, cheat, or steal, or tolerate those who do."

Upon accepting admission to Texas A&M University, a student immediately assumes a commitment to uphold the Honor Code, to accept responsibility for learning, and to follow the philosophy and rules of the Honor System. Students will be required to state their commitment on examinations, research papers, and other academic work. Ignorance of the rules does not exclude any member of the TAMU community from the requirements or the process of the Honor System. Additional information about the Aggie Honor Code can be found at: http://www.tamu.edu/aggiehonor/. The consequences for cheating and plagiarism on any assignment will result in an unsatisfactory grade for the course.