Fall 9-1-2021

CHMY 562.01: Organic Structure and Mechanism

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Syllabus and Tentative Course Outline for CHMY 562
Organic Structure and Mechanism
(CRN 73792) Autumn 2021

Lectures: **Monday 9:00am to 12:00pm; Room CHEM 204**

Instructor: Orion B. Berryman email: orion.berryman@umontana.edu office: 207 CHEM

Office Hrs: **By appointment 207 CHEM**

Text: *Modern Physical Organic Chemistry,* Eric V. Anslyn and Dennis A. Dougherty, University Science Books: Sausalito, CA; 2006 (Required)
Text Website: http://www.uscibooks.com/anslyn.htm

Other Texts: *Mechanism and Theory in Organic Chemistry*, Lowry & Richardson
Advanced Organic Chemistry, Part A, Carey & Sundberg
Supramolecular Chemistry, Second Edition, J. W. Steed and J. L. Atwood
Physical Methods for Chemists, Drago

Websites: https://moodle.umt.edu/
http://www.chem.wisc.edu/areas/organic/index-chem.htm
pka's: http://www.chem.wisc.edu/areas/reich/pkatable/index.htm
http://ccc.chem.pitt.edu/wipf/MechOMs/evans_pKa_table.pdf
https://diverdi.colostate.edu/C477/miscellanea/CRC%20reference%20data/dissociation%20constants%20of%20organic%20acids%20and%20bases.pdf

Grading:		
	Ten Homework Sets/Participation (half P/N)	100 points
	80-Minute Midterm Exam week of October 10th	100 points
	80-Minute Midterm Exam week of November 8th	100 points
	Student Lit. Present. Week of November 29th	50 points
	Computational Chemistry Project	50 points
	Comprehensive Final Examination	
	TBD	200 points
	Total	**600 points**

Student Literature Presentation: Find a recent paper in the chemical literature in the broadly defined field of physical organic chemistry (I recommend finding something in *JACS*, *Angew. Chem.* or *Nature Chem.*).

- In class presentation (15 minutes):
- Provide a written short summary of the paper and written suggested exam or quiz question from your selected paper. If this question is used on an exam or HW, you will receive 10 bonus points.

CHMY 562 – Organic Structure and Mechanism

***Tentative* Course Timetable for CHMY 562**

➔ Brief listing of *selected* topics to be covered.

Week 1: Week of August 30th

Review – Prequiz, VSEPR, hybridization, MO description; polar bonds and dipoles; resonance, bond lengths and polarizability (1.1); carbocations, radicals, carbanions and carbenes; relative stability, electron delocalization (1.4)

Week 2: Week of September 6th (Labor Day, September 6)

Bonding review (CH 1.1 and 1.4) – VSEPR, hybridization, MO description; polar bonds and dipoles; resonance, bond lengths and polarizability (1.1); carbocations, radicals, carbanions and carbenes; relative stability, electron delocalization (1.4). HW #1

***Week 3: Week of September 13th* (HW #1 DUE)**

Bonding review, cont.

Acid-Base Chemistry (CH 5) – homolytic vs. heterolytic bond cleavage, aqueous and non-aqueous systems; predicting pKa's (5.1-5.4). HW #2

***Week 4: Week of September 20th* (HW #2 DUE)**

Acid-Base Chemistry, cont. – solvent effects; HSAB theory/relative nucleophilicity and electrophilicity (5.6); biologicial examples and non-solvent influences on pKa (5.5). HW #3

***Week 5: Week of September 27th* (HW #3 DUE)**

Strain and Stability (CH 2) – Thermochemistry: types of energy, energy surfaces, strain energy (2.1); BDEs, group increments and radical stability (2.1.3, 2.2). HW #4

***Week 6: Week of October 4th* (HW #4 DUE)**

Strain and Stability (CH 2), cont. – conformational analysis, A-values, electronic effects, aromaticity (2.3, 2.4). HW #5

***Week 7: Week of October 11th* (HW #5 DUE)**

Midterm Exam #1

Strain and Stability (CH 2), cont.

Noncovalent Interactions and Solvation Effects (CH 3) – solvent properties and thermodynamics (3.1); "weak" interactions: H-bonds, dipole interactions, pi interactions, solvophobic effects, etc. (3.2 + additional reading) HW #6

***Week 8: Week of October 18th* (NO HW DUE)**

Noncovalent Interactions and Solvation Effects (CH 3), cont. – "weak" interactions, cont.

***Week 9: Week of October 25th* (HW #6 DUE)**

Molecular Recognition and Supramolecular Chemistry (CH 4) – thermodynamics of binding/association, binding isotherms, measuring Ka's (4.1); Molecular Recognition: complementarity, preorganization, hydrophobic effects, examples from the literature (4.2); Supramolecular Chemistry and Self-Assembly: modern examples of physical organic chemistry in confined spaces (4.3). HW #7

***Week 10: Week of November 1st* (HW #7 DUE)**

Literature Review Topics Due

Molecular Recognition and Supramolecular Chemistry (CH 4), cont. – binding interactions, cont. HW #8

***Week 11: Week of November 8th (Veterans Day, November 11th)* (HW #8 DUE)**

Midterm Exam #2

Read: An Introduction to Computational Chemistry (CH 2.6) *Read: Computational Chemistry III (CH 14.1, 14.2) – ab initio, semi-empirical and density functional theory (14.1, 14.2).* HW #COMP

CHMY 562 – Organic Structure and Mechanism

Week 12: Week of November 15th **(HW #COMP DUE)**

Transition State Theory (CH 7) – energy surfaces and TST (7.1, 7.2); kinetics: Hammond Postulate, reactivity vs. selectivity principle, Curtin-Hammett Principle, microscopic reversibility, experimental determination (7.3, 7.4); steady state kinetics (7.5). HW #9

Week 13: Week of November 22nd (Thanksgiving, November 24-26th) **(HW #9 DUE)**

Catalysis (CH 9) – Transition state binding (9.1); forms of catalysis (9.2); Bronsted acid-base catalysis; **Time permitting – Organic Reaction Mechanisms (CH 10/11)** – Predicting organic reactivity (10.1); Hydration of carbonyl structures (10.2). HW #10

Week 14: Week of November 29th **(HW #10 DUE)**

Student Literature Presentations

Week 15: Week of December 6th

➔ **FINAL Exam: TBA**

➔ *This is a rough outline. Time permitting we will cover selected topics in Chapters 9, 10 & 11.*