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CHMY 562.01: Organic Structure and Mechanism

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Syllabus and Tentative Course Outline for CHMY 562
Organic Structure and Mechanism
(CRN 74660) Autumn 2020

Lectures: **Wednesday 12:00pm to 2:50pm; 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/login/index.php
http://www.chem.wisc.edu/areas/organic/index-chem.htm
pka's: http://www.chem.wisc.edu/areas/reich/pkatable/index.htm
http://www2.lsdiv.harvard.edu/labs/evans/pdf/evans_pKa_table.pdf
http://rwindigo1.chm.colostate.edu/c545/pKa.values.pdf

Grading:		
	Homework Sets/Participation	half P/N 100 points
	80-Minute Midterm Exam week of September 28th	100 points
	80-Minute Midterm Exam week of October 26th	100 points
	Student Lit. Present. Week of November 16th	100 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 17th

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 August 24th

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)

Week 3: Week of August 31st

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)

Week 4: Week of September 7th (Labor Day September 7th)

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

Week 5: Week of September 14th

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)

Tentative Read: An Introduction to Computational Chemistry (CH 2.6)

Week 6: Week of September 21st

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

Week 7: Week of September 28th

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)

Week 8: Week of October 5th

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

Week 9: Week of October 12nd

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

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)

Week 10: Week of October 19th

Literature Review Topics Due

Self-Assembly (Supramolecular Chemistry CH 10) – Proteins and foldamers, kinetics vs thermodynamics, coordination compounds, hydrogen bonding complexes, catenanes and rotaxanes

CHMY 562 – Organic Structure and Mechanism

Week 11: Week of October 26th (Halloween, October 31)

Midterm Exam #2

Supramolecular Catalysis (Supramolecular Chemistry CH 11) – Biological mimics, cyclodextrins, cation binding hosts, metallobiosites, abiotic supramolecular catalysis, dynamic covalent libraries, self-replicating systems, emergence of life?

Week 12: Week of November 2nd (Election Day, November 3rd)

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)

Read: Computational Chemistry III (CH 14.1, 14.2) – ab initio, semi-empirical and density functional theory (14.1, 14.2)

Week 13: Week of November 9th (Veterans Day November 11th: Alternative class day?)

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); other topics as time permits

Week 14: Week of November 16th

Student Literature Presentations

Week 15: Week of November 23rd

➔ **FINAL Exam: TBA**

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