Chem 2513: Introductory Organic Chemistry I

Instructor/Contact	FA01 (8:30 am): Teri Gullon, teri.gullon@acadiau.ca FA02 (9:30 am): Dr. Amitabh Jha, amitabh.jha@acadiau.ca
Office and Office Hours	Teri Gullon: MWF 9:20-10 am and Via Teams Dr. Amitabh Jha: Wednesdays 1.30-4.30 pm (Teams/In person)
Lecture	MWF 8:30-9:25 am (Section 1 – BAC 239) MWF 9:30-10:25 (Section 2 – ELL 207)

Book (Optional): ***Organic Chemistry*** by David Klein, J Wiley and Sons. Any edition of the text is acceptable. Another recommended/alternative book: ***Organic Chemistry as a Second Language*** (1^{st} semester topics) by David Klein. The full textbook is strongly recommended if you intend on taking additional organic chemistry courses.

Description: This is an introductory course in organic chemistry. Topics to be examined include organic structure and nomenclature (alkane, alkene, alkyne, alcohols, alkyl halides, alcohols), basic functional groups and IR spectroscopy, isomerism, stereochemistry, and an introduction to synthesis, reactions and reaction mechanisms. Structure and function will be emphasized. The lecture portion does not require the students to bring their laptops although taking notes is highly recommended.

Topics:
1 – Molecular bonding, structure and resonance theory
2 – Polarity, functional groups and IR spectroscopy
3 – Acid/base theory and mechanism
4 – Nomenclature and conformations of alkanes, ^{13}C NMR spectroscopy
5 – Stereochemistry
6 – Ionic reactions: substitution and elimination
7 – Alkenes and alkynes I, properties and synthesis
8 - Alkenes and alkynes I, addition reactions
9 – Radical reactions
10 – Alcohols and ethers

Requirements: The prerequisite for this course is CHEM 1023 or CHEM 1123 with a minimum grade of C-. Since chemistry is a laboratory science, the laboratory for this class is an integral part of the course. You must obtain a passing grade in the laboratory to pass the course.

Lab attendance is mandatory. Missing more than two labs (with or without permission) results in an automatic fail for the lab portion (and the course as a result). Notify the lab instructor **as soon as possible** if you are ill or unable to attend an upcoming lab, so that a makeup lab can be arranged (makeup labs are not always possible). If the instructor is not notified **prior** to the lab period, a grade of zero will be assigned for the missed work.

Course Material:
REQUIRED: Lab coat, safety glasses and lab manual and notebook
RECOMMENDED: Textbook (Klein), Molecular Model Kit

Grading	Assignments (ACORN) 5% Class Quizzes (based on homework) 5% Labs 20% Tests (2) 15 each = 30% Final Exam 40%

Organization: Lectures will be delivered live in-person. Masks are required for the duration of the lecture. Please refrain from moving around the lecture halls and maintain social distancing if possible.

There are two types of practice for grades. ACORN (multiple choice) assignments (one per module) which will be due a week after BOTH sections complete the topic. And in-class quizzes which are selected from previously posted homework on ACORN. These are completed in-class and will consist of 1-2 questions selected from the Module homework already posted on ACORN (NOT the same as the ACORN assignments).

No make up tests will be given in this course. If you feel you have a valid reason for missing a test, please send the documents to Registrar's office. **Only Registrar's note of excuse will be accepted for all course work**. A missed test with no valid reason by the deadline will count as zero. An excused test will be eligible for replacement with the final examination grade. Only ONE midterm test may be replaced in this way. The course will terminate in a written 3 h examination date TBA.

Both in-class quizzes and the written portion of the tests will be uploaded to the website Gradescope.ca. The onus is on the student to ensure documents are visible and complete upon uploading. Instructions on converting into a SINGLE PDF are on ACORN.

Please note that the organization of the course may be subject to change due to COVID-19 restrictions.

Miscellaneous: The ACORN site has additional resources including video lectures. Note: these recorded lectures do not cover the exact same information and **<u>are not</u>** a substitute for attending class.

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Test Dates:
TBD

Grading Scheme

A+: 90-100	B+: 77-79	C+: 67-69	D+: 57-59	
A : 85-89	B : 73-76	C : 63-66	D : 53-56	
A-: 80-84	B-: 70-72	C-: 60-62	D-: 50-52	F: <50

Accessible Learning Services: Acadia University is dedicated to improving access to campus life for all students with disabilities. While we attempt to ensure that all courses are accessible, we recognize that there are barriers that need to be addressed on an individual basis. Students who require accommodations to complete coursework or otherwise fully participate in class should contact Accessible Learning Services directly as soon as possible. Please visit Accessible Learning Services website or email them at accessible.learning@acadiau.ca for more information.

Detailed List of Topics and Learning Objectives

Module 1: Review of Bonding and Molecular Structure

a) Electron Configurations
b) Atomic orbitals, hybridization, and Valence Bond Theory
c) Lewis structures, resonance, molecular shapes
d) Condensed structural and bond-line formulas
e) Constitutional Isomers

Objectives:

- Review material from Introductory Chemistry (atomic structure, electronic configurations)
- Learn and practice how to draw Lewis structures and molecular shape
- Understand the basics of hybridization to be able to identify respective hybridization of atoms
- Fully understand resonance theory and be able to draw resonance structures of a molecule including arrow pushing of electrons

Module 2: Functional Groups and IR Spectroscopy

a) Electronegativity and polarity
b) Intermolecular forces in organic molecules
c) Survey of common organic functional groups and their physical properties
d) Introduction to IR spectroscopy
e) Identification of common organic functional groups with IR spectroscopy

Objectives:

- Identify polar molecules

- Rank compounds physical characteristics (boiling point, melting point) using intermolecular forces
- Identify and name functional groups on molecules
- Interpret and Infra-red spectrum, assign stretches, match molecules to IR spectra

Module 3: Acids, Bases and Mechanisms

a) Arrhenius, Bronsted Lowry, and Lewis definitions of acids and bases
b) Use of Curved arrows
c) Strong acids and bases and the leveling effect
d) Weak acids and use of pK_a as measure of acid strength
e) Factors controlling acid strength (inductive, resonance, sterics, EN, hybridization)
f) Organic functional groups as bases
g) Lewis acids and bases in Organic chemistry: introduction of nucleophiles and electrophiles
h) Carbon-centered electrophiles (carbocations) and nucleophiles (carbanions)

Objectives:

- Define acids and bases
- Understand different effects (inductive, resonance, sterics, hybridization) on stability
- Predict acid/base strength
- Predict which way an equilibrium lies
- Understand meaning of pKa

Module 4: Alkanes

a) Properties of linear, branched, and cyclic alkanes and nomenclature
b) Structure, bonding, and hybridization in alkanes
c) Alkane stability as function of structure
d) Introduction to oxidation and reduction of carbon atoms in organic compounds
e) Conformations of alkanes (staggered vs eclipsed) and Newman projections
f) Strain in alkyl chains and rings (angle strain, torsional strain, van der Waals strain)
g) Conformations of cyclic alkanes, chair/boat conformations of cyclohexane, chair flipping
h) Stereoisomerism in cycloalkanes
i) Introduction to carbon-13 NMR spectroscopy
j) Identification of common signals in carbon-13 NMR spectroscopy

Objectives:

- Be capable of naming molecules following IUPAC rules
- Understand and predict the boiling/melting points of alkanes based on intermolecular forces
- Be able to draw Newman projections
- Understand ring strain
- Draw cyclohexane in both flat and chair methods
- Be able to draw a cyclohexane chair structure many different ways, including with ring flips
- Predict relative stability of conformers
- Identify cis/trans isomers
- Predict number and environment of ^{13}C NMR signals

Module 5: Stereochemistry

a) Introduction to chirality
b) Stereoisomerism: enantiomers vs diastereomers
c) Properties of enantiomers, optical rotation and specific rotation
d) Absolute and relative configurations, measurement of optical purity
e) CIP rules for assigning absolute configurations (R and S)
f) Planes of symmetry, meso compounds
g) Fischer projections

Objectives:

- Be capable of assigning R/S to chiral centers
- Understand and identify the stereochemical relationship between molecules (enantiomers/diastereomers)
- Know when and why a molecule is optically active
- Be fluent in the terminology associated with this module

Module 6: Ionic Reactions

a) Review of reaction mechanism, potential energy diagrams, reaction coordinates
b) S_N2 reactions: mechanism, stereospecificity, rates
c) S_N1 reactions: mechanism, stereospecificity, rates
d) Carbocation stability
e) Factors influencing competition between S_N1 and S_N2
f) E1 reactions: mechanism, stereospecificity, rates
g) E2 reactions: mechanism, stereospecificity, rates
h) Factors influencing competition between E1, E2, S_N1, and S_N2

Objectives:

- Become comfortable with the terminology associated with this module
- Understand and draw the mechanisms of S_N1, S_N2, E1 and E2
- Be able to identify a mechanism based on Free Energy diagrams
- Understand the principles of nucleophile strength, electrophile, leaving group strength and steric effects
- Be able to predict which reaction pathway dominates

Module 7: Alkenes and Alkynes

a) Structure, bonding, and hybridization in alkenes
b) Stereoisomerism in alkenes and CIP rules (E vs Z)
c) Alkene stability
d) Preparation of alkenes 1: dehydrogenation
e) Preparation of alkenes 2: dehydration (full mechanistic discussion)
f) Regioselectivity and Zaitsev's rule
g) Rearrangements of carbocations
h) Preparation of alkenes 3: dehydrohalogenation (full mechanistic discussion)
i) Hoffman's rule
j) anti-periplanar rule in E2

k) Properties and bonding in alkynes
l) Preparation of alkynes from vicinal dihalides (full mechanistic discussion)
m) Acidity of terminal alkynes and nucleophilicity of alkynides

Objectives:

- Be capable of naming various functionalized alkenes and cycloalkenes including stereoisomers
- Be able to draw complete dehydration mechanisms and predict when they occur
- Better understand and be able to identify the mechanisms and products of specific reaction conditions
- Correctly identify β-hydrogens necessary for elimination mechanisms, including those off of cyclohexane rings
- Predict reaction products keeping in mind rearrangements and the Zaitsev and Hoffmann rules
- Synthetically understand alkyne formation and deprotonation, and alkyne anions use as nucleophiles

Module 8: Addition Reactions

a) Hydrogenation of alkenes (mechanism, syn stereochemistry)
b) Hydrogenation of alkynes using transition metal and poisoned catalysts
c) Dissolving metal reduction of alkynes to *trans*-alkenes
d) Electrophilic addition of HX to alkenes (mechanism)
e) Markovnikov's rule
f) Acid catalyzed hydration of alkenes (mechanism)
g) Oxymercuration-demercuration of alkenes
h) Hydroboration-oxidation of alkenes (mechanism, stereochemistry)
i) Addition of X_2 to alkenes, bromonium/chloronium ions (mechanism, anti stereochemistry)
j) Addition of X_2 to alkenes in presence of nucleophiles (mechanism, regio/stereochemistry)
k) Preparation of cyclopropanes via carbene addition to alkenes (mechanism)
l) Preparation of vicinal diols from alkenes (OsO_4 or $KMnO_4$ oxidation)
m) Oxidative cleavage of alkenes (hot $KMnO_4$ or ozonolysis)
n) Addition of X_2 to alkynes
o) Addition of HX to alkynes
p) Multistep organic synthesis

Objectives:

- Predict the products for the addition reactions outlined in this module
- Draw complete mechanisms for the addition reactions which were covered (you are not responsible for all the mechanisms, refer to the final slide to be sure which ones you need to know)
- Keep in mind stereochemistry and regioselectivity when predicting products

Module 9: Radical Reactions

a) Heterolysis vs homolysis

b) Free radical stability
c) Radical mechanisms (initiation, propagation, termination)
d) Radical halogenation of alkanes (mechanism)
e) Radical polymerization (mechanism)

Objectives:

- Understand the basics of radical chemistry theory
- Be capable of writing full radical mechanisms for the radical halogenation and HBr addition as well as polymerization reactions
- Be capable of differentiating between initiation, propagation and termination steps in a mechanism
- Predict radical stability and stereochemical outcomes of radical reactions

Module 10: Alcohols and Ethers

a) Halogenation of alcohols using PX_3 (mechanism and stereochemistry)
b) Preparation of sulfonate esters (OTs, OMs, OTf) from alcohols
c) Sulfonate esters as leaving groups (mechanism and stereochemistry).
d) Acid/base properties of alcohols
e) Williamson ether synthesis (mechanism)
f) Protecting groups in organic synthesis
g) Protection of alcohols as silyl ethers
h) Deprotection of silyl ethers using TBAF
i) Epoxidation of alkenes using peroxyacids (mechanism and stereochemistry)
j) Preparation of epoxides from vicinal halohydrins
k) Acid and base catalyzed ring opening of epoxides

Objectives:

- Name and identify alcohols and ethers
- Convert alcohols into better leaving groups using various methods
- Understand what protecting groups are, and when to use them
- Learn two ways to make epoxides, and two condition sets to open them