

**UNIVERSITY OF CALGARY
FACULTY OF SCIENCE
DEPARTMENT OF CHEMISTRY
COURSE SYLLABUS
WINTER 2017**

1. Course: CHEMISTRY 351, Organic Chemistry I

LEC	DAYS	TIME	ROOM	INSTRUCTOR	OFFICE	EMAIL	OFFICE HOURS
L01	MWF	10:00-10:50	ES 162	Dr. Wendy Benoit	EEEL 235A	wbenoit@ucalgary.ca	TBA

Desire 2 Learn (D2L) : CHEM 351 L01 - (Winter 2017) – Organic Chemistry I

Course website: <http://www.chem.ucalgary.ca/courses/350/index351-w17.html>

Departmental Office: Room SA 229, Tel: 403-220-5341, e-mail: uginfo@chem.ucalgary.ca

2. Course Description:

An introduction to Organic Chemistry from a mechanistic perspective. Structure, bonding, and function, e.g. physical properties and reactivity. Stereochemistry, kinetics and thermodynamics, spectroscopy (nuclear magnetic resonance, infrared, ultra-violet/visible, and mass spectrometric techniques). Substitution and elimination reactions of saturated functional groups - the chemistry of alkanes, alkyl halides, alcohols and their derivatives. Laboratory: Practical techniques.

3. Recommended/ Required Textbook(s): No textbook is required for this course. Students can access the etext available free of charge through the course website (<http://www.chem.ucalgary.ca/courses/351/Carey5th/Carey.html>).

4. Topics Covered and Suggested Readings:

Course Content

Fundamentals of Structure and Bonding and the Language of Organic Chemistry

Bonding: ionic, covalent, polar covalent bonds, dipoles, etc.
 Lewis structures of organic molecules
 Language of organic chemistry (types of arrows, types of diagrams e.g. wedge-hash, Newman, Fischer)
 VSEPR (shapes of molecules)
 Introduction to MO theory (orbitals in molecules = where the electrons are)
 Hybridisation of simple molecules: hydrocarbons, expand to functional groups
 Formal charge (review, examples of common organic situations)
 Oxidation state (review, examples of common organic situations)
 Using curly arrows (rules for drawing/checking/applications)
 Resonance (definition, reasoning for use, implications on structure/reactivity)
 pKa trends (organic acids and bases, related to structure, factors affecting each, introducing enolates)
 Bond properties (energies, lengths)
 Hydrocarbons: types alkanes, alkenes, alkynes, arenes; saturated, unsaturated, IHD
 Isomers (drawing, constitutional, conformational, configurational, geometric, optical, enantiomers, diastereomers)
 Intermolecular forces and physical properties (e.g. mp, bp, solubility)
 Thermodynamic stability: heats of combustion, heats of formation, using Hess's Law
 Conformational analysis: terminology
 Conformational analysis of alkanes and cycloalkanes
 Conformational analysis of substituted cycloalkanes
 Nomenclature of organic compounds (including stereoisomers e.g. E/Z and R/S terminology)

Chapter in etext

(not all sections will be covered)

Chapters 1-4, 7

For nomenclature:

Can refer to Chapter 2-6, 9, 11, 14-24 for general information on naming and reactivity of each functional group (Chapter names match the functional group names, e.g. "Chapter 4 – Alcohols and alkyl halides")

Course Content (continued)

Chapter in text
(not all sections will be covered)

Spectroscopy and related techniques

Elemental analysis

Infrared spectroscopy: principles, Hooke's law model, vibrational modes, polar bonds, characteristic functional group stretches

Mass spectrometry: principles, molecular ion, simple fragments, isotope patterns for Cl and Br

^1H NMR spectroscopy: principles, types of H, chemical shift, integration, simple coupling patterns, complex coupling in alkenes and benzenes

^{13}C NMR spectroscopy: broad band decoupled, compare and contrast with ^1H NMR spectroscopy.

Using spectroscopic data to deduce structure

Chapter 13

Reactions

Radical substitution reactions of alkanes to give alkyl halides

Radicals (stability factors and trends)

n.b. allylic and benzylic radical substitutions

Chapter 4-5, 8-9, 15

Nucleophilic substitution reactions of alkyl halides and alcohols (and related systems e.g. thiols, ethers, amines)

$\text{S}_{\text{N}}1$ mechanism (kinetics, key factors affecting $\text{S}_{\text{N}}1$, stereochemistry)

Carbocations (stability factors and trends)

$\text{S}_{\text{N}}2$ mechanism (kinetics, key factors affecting $\text{S}_{\text{N}}2$, stereochemistry)

Nucleophilicity (factors and trends)

Leaving groups (factors and trends)

Reactions of alkyl halides with common nucleophiles (including acetylides, enolates, etc.)

Reactions of alcohols with HX, PX_3 , SOCl_2 etc.

Preparations and reactions of tosylates (as a good leaving group)

Ether synthesis (using alcohols or phenols)

Elimination reactions of alkyl halides (dehydrohalogenation) and alcohols

(dehydration) to give alkenes Alkenes: stability trends based on

thermodynamic data (e.g. heats of hydrogenation) related to structure (degree of substitution, E or Z)

Zaitsev's rule

E_1 mechanism

Carbocation rearrangements (via 1,2-hydride and 1,2-alkyl shifts)

E_2 mechanism

E_2 stereochemistry implications in cyclic systems

E_1cB mechanism

Alkynes from elimination reactions

Basicity vs. nucleophilicity

Substitution vs. eliminations (factors that influence the major pathway)

Application of reactions to the synthesis of organic molecules

Course Learning Outcomes:

By the end of this course, students will be expected to:

- Recognize and employ the conventions of naming, structure drawing, and curved arrow pushing to communicate about organic compounds.
- Draw reaction mechanisms with appropriate curved arrows to account for how bonds are made and broken in organic reactions
- Analyze the structural features of starting materials, reaction intermediates, and products to predict or rationalize their physical properties or reaction behaviour.
- Identify and interpret spectral data to deduce the structure of simple organic molecules.
- Perform laboratory experiments using techniques that are safe and appropriate for handling and manipulating organic compounds.
- Propose a short (ca. 1-4 step), feasible synthesis for the formation of a specific organic product using a limited number of possible reaction types: acid/base, radical substitution, nucleophilic substitution, or elimination reactions.

4. Laboratory Experiments: (10 weeks, 3 hours/ week)

1. Solubility of Organic Compounds
2. Melting point and Boiling point determination
3. Molecular Models (structure and bonding)
- 4a and b. (2 week experiment) Synthesis of Analgesics (i) acetaminophen and (ii) aspirin
5. Reactivity of Hydrocarbons
6. Spectroscopy
7. Isolation of a Natural Product: Caffeine
8. Chromatography
9. Reactivity in Substitution Reactions

Department Approval: Approved by Department Head

Date: December 16, 2016