UNIVERSITY OF CALGARY
DEPARTMENT OF CHEMISTRY
COURSE SYLLABUS
WINTER 2015

COURSE: CHEMISTRY 351, Organic Chemistry I

LEC	DAYS	TIME	ROOM	INSTRUCTOR	OFFICE	PHONE	EMAIL	OFFICE HOURS
L01	MWF	10:00-10:50	ICT 102	Dr. W. L. Benoit	EEEL 235A	220-3652	wlbenoit@ucalgary.ca	TBA
Laboratory Coordinator:				Dr. W. L. Benoit	EEEL 235A	220-3652	wlbenoit@ucalgary.ca	TBA

TEXTBOOK AND OTHER RECOMMENDED MATERIALS FOR THE COURSE: (available from the Bookstore)

M. Jones, S.A. Fleming, "Organic Chemistry", Norton 4th ed. 2010 or 5th ed. 2014
M. Jones, H.L. Gingrich, S.A. Fleming, "Study Guide / Solutions Manual", Norton 4th ed. 2010. or 5th ed. 2014
Molecular Models: *very strongly* recommended (allowed resource on examinations)
Chemistry 351 Laboratory Manual (on-line, downloadable pdf files from course website)
A self-duplicating Laboratory Notebook
Top Hat Monocle registration (available from Top Hat Monocle, see course website for more details)

TOPICS COVERED:

Chemistry 351 is an introduction to organic chemistry and spectroscopy, discussing the fundamental concepts required to understand organic chemistry based on a mechanistic approach. This will involve discussing bonding and molecular structure and the implications these have on the properties and reactivity of organic molecules.

Fundamentals
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)
pKa trends (organic acids and bases, related to structure, factors affecting each, introducing enolates)
Bond properties (energies, lengths)
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)
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

Spectroscopy and related techniques
Elemental analysis
Infrared spectroscopy: principles, Hookes law model, vibrational modes, polar bonds, characteristic functional group stretches

Mass spectrometry: principles, molecular ion, simple fragments, isotope patterns for Cl and Br
^{1}H 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 ^{1}H NMR spectroscopy.
Using spectroscopic data to deduce structure

Reactions
Radical substitution reactions of alkanes to give alkyl halides
Radicals (stability factors and trends)
n.b. allylic and benzylic radical substitutions

Nucleophilic substitution reactions of alkyl halides and alcohols (and related systems e.g. thiols, ethers, amines)
SN1 mechanism (kinetics, key factors affecting SN1, stereochemistry)
Carbocations (stability factors and trends)
SN2 mechanism (kinetics, key factors affecting SN2, 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 (dehydrohalgenation) 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)
Zaitsevs rule
E1 mechanism
Carbocation rearrangements (via 1,2-hydride and 1,2-alkyl shifts)
E2 mechanism
E2 stereochemistry implications in cyclic systems
E1cB mechanism
Alkynes from elimination reactions

General
Nomenclature of organic compounds (including stereoisomers e.g. E/Z and R/S terminology)
Basicity vs. nucleophilicity
Substitution vs. eliminations (factors that influence the major pathway)
Application of reactions to the synthesis of organic molecules

LABORATORY EXPERIMENTS: (10 weeks of experiments)
Solubility of Organic Compounds
Melting point and Boiling point determination
Synthesis of Analgesics (i) acetominophen and (ii) aspirin
Molecular Models (structure and bonding)
Reactivity of Hydrocarbons
Isolation of a Natural Product: Caffeine
Spectroscopy
Reactivity in Substitution Reactions
Chromatography