



## UNIVERSITY OF CALGARY

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DEPARTMENT OF CHEMISTRY

### Chem 351 Syllabus Fall 2017

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.

#### Basics

Bonding : ionic, covalent, polar covalent bonds, dipoles *etc.*

Lewis structures of organic molecules

Language of organic chemistry (what do all the arrows mean, diagrams (wedge-hash, Newman, Fischer *etc.*)

pKa trends (organic acids and bases, related to structure, factors affecting each inc. introducing enolates)

Bond properties (energies, lengths)

VSEPR (shapes of molecules)

Introduction to MO theory (orbitals in molecules = where the electrons are)

Hybridisation in 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 (what? why? Implications on structure / reactivity)

Hydrocarbons : types of: alkanes, alkenes, alkynes, arenes. Saturated or unsaturated ? IHD

Isomers (drawing, constitutional, conformational, configurational, geometric, optical, enantiomers, diastereomers)

Intermolecular forces and physical properties (*e.g.* mpt, bpt, 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

Infra red: principles, Hooke's law model, vibrational modes, polar bonds, characteristic FG stretches

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

<sup>1</sup>H NMR: principles, types of H, chemical shift, integration, simple coupling patterns, complex coupling in alkene and benzene systems.

<sup>13</sup>C NMR: broad band decoupled, compare and contrast with <sup>1</sup>H NMR.

Using spectroscopy to deduce structure

Continued

## Chem 351 Syllabus (continued)

### Reactions

**Radical substitution reactions** of alkanes to give alkyl halides. (*n.b.* inc. allylic and benzylic radical subs)  
Radicals (stability factors related to structure and overall trends)

**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 related to structure and overall trends)  
SN2 mechanism (kinetics, key factors affecting SN2, stereochemistry)  
Nucleophilicity (structural factors and trends)  
Leaving groups (structural factors and trends)  
Reactions of alkyl halides with common nucleophiles (inc. acetylides, enolates *etc.*)  
Reactions of alcohols with HX, PX<sub>3</sub>, SOCl<sub>2</sub> *etc.*  
Preparations & reactions of tosylates (as a better leaving group)  
Ether synthesis (from both alcohols and phenols)

**Elimination reactions** of alkyl halides (dehydrohalogenation) and alcohols (dehydration) to give alkenes  
Alkenes : stability trends based on heats of hydrogenation *etc.* related to structure (degree of subs, E or Z)  
Zaitsev's rule  
E1 mechanism  
Carbocation rearrangements (via 1,2-hydride and 1,2-alkyl shifts)  
E2 mechanism  
E2 stereochemistry implications in cyclic systems *etc.*  
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) acetaminophen and (ii) aspirin  
Molecular Models (structure and bonding)  
Isolation of a Natural Product : Caffeine  
Chromatography  
Reactivity of Hydrocarbons  
Spectroscopy  
Reactivity in Substitution Reactions