UNIVERSITY OF CALGARY
DEPARTMENT OF CHEMISTRY

Chem 351 Syllabus FALL 2023

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)
Hybridization 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 (IR): principles, Hooke's law model basic idea, vibrational modes, polar bonds, characteristic FG stretches

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

^{1}H NMR: principles, types of H, chemical shift, integration, simple coupling patterns, complex coupling in alkene and benzene systems.

^{13}C NMR: broad band decoupled, compare and contrast with ^{1}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_3, $SOCl_2$ *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: (A laboratory orientation, followed by 8 weeks of tentative experiments)

- this list and order of experiments may change, please see the course website for the most up to date list.

1. Solubility of Organic Compounds
2. Recrystallization
3. Melting point and Boiling point determination
4. Molecular Models (structure and bonding)
5. Synthesis of Analgesics
6. Isolation of a Natural Product : Caffeine
7. Chromatography
8. Reactivity in Substitution Reactions