UNIVERSITY OF CALGARY
DEPARTMENT OF CHEMISTRY

Chem 559 Syllabus Fall 2021

Goals: By the end of this course, students will be expected to be able to interpret and use the spectroscopic data from UV, MS, IR and NMR (including 2D) spectra to be able to (a) distinguish similar structures or (b) deduce the structure of an unknown organic molecule.

Introduction
- Course goals
- Review of principles / trouble spots from prerequisites

Deducing structure from spectra – application of the fragment approach to spectroscopic problem solving

Ultra-violet / visible spectroscopy
- Basic instrumentation principles
- Beer Lambert Law
- Forbidden and allowed transitions
- Chromophores : structural and solvent effects, including orbital perspective
- Rules for predicting λmax for dienes, enones, polyenes and aromatic systems

Mass spectroscopy
- Basic instrumentation principles including overview of different ionisation techniques
- Nitrogen rule
- Isotope patterns (13C, halogens Cl and Br including polyhalogenated *etc*.)
- Typical fragmentation & rearrangement pathways of common functional groups with mechanistic analysis

Infra-red spectroscopy
- Basic instrumentation principles
- Hooke's Law model of molecular vibrations
- Vibrational modes and coupled vibrations
- Functional group charateristic frequencies
- Structural effects on vibrational frequencies (hydrogen bonding, conjugation, ring strain, aromatic substitution patterns, tautomerism)

Nuclear Magnetic Resonance spectroscopy
- Basic instrumentation principles
- NMR active nuclei
- Factors that influence chemical shift (electronegativity, anisotropy, sample conditions)
- Spin system notation (Pople)
- Chemical and magnetic equivalence (topicity)
- Homo- and heteronuclear coupling
    - Splitting diagrams
    - Strong (2nd order) and weak (1st order), effect of $\Delta\nu/J$ on observed coupling pattern
    - Typical coupling constants J for 2-, 3- and longer range coupling
    - Mechanism of coupling
    - Karplus equations
- Dynamic NMR (conformational, tautomeric *etc*.)
- Methods for calculating chemical shifts (H and 13C NMR)
- C NMR (broadband, off resonance, APT, DEPT)
- NOE effect and spectroscopic methods
- Correlation (2D) spectroscopy (especially H / H, H / C and C / C methods).