UNIVERSITY OF CALGARY
DEPARTMENT OF CHEMISTRY

Chem 559 Syllabus Fall 2015

Deducing structure from spectra - the fragment approach to spectroscopy 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 (esp. H / H, H / C and C / C methods)

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