Camosun College

Department of Chemistry and Geoscience

Chemistry 213 Fall 2002

Molecular Spectroscopy

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Texts and supplies:

"Practical Spectroscopy" by P. R. Young

"Chemistry 213 Laboratory Manual and Study Guide" by C.G.C.Shorthill

These items are available in the bookstore. In addition, there are several organic and inorganic texts which contain excellent sections on molecular spectroscopy, notably: Solomons, Fessendon and Fessendon, etc. Students have such books from other courses and they are encouraged to read the appropriate sections. Moreover, there are several books that are held on reserve for you in the library that can be signed out for limited periods at the front desk.

Supplementary handouts will be given at appropriate times throughout the semester.

Students should obtain a green duotang binder for laboratory reports and have a scientific calculator for all numerical work in this course.

It is a departmental requirement that all students working in a laboratory must wear safety glasses. Students, who normally do **not** wear spectacles, must obtain a pair for themselves before they begin the laboratory experiments.

Assessment:

The final grades for the course will be assigned on the basis of the following:

Mid term examination (1)	10%
Mid term examination (2)	25%
Final examination	40%
Laboratory	25%

Grades:

The following percentages refer to the composite total obtained at the end of the course .

A range	85% to 100%
B range	70% to 84%
C range	60% to 69%
D range	50% to 59%
F range	<50%

Note: This table is given only as a guide and the exact equivalency will be determined by the instructor when all the marks are available. In cases where there is a major difference between the mark on the final examination and the composite total, the instructor reserves the right to adjust the final grade to reflect this difference. The passing grade is C and to pass the course, students must obtain passing grades in both the lecture and laboratory portions of it.

Course content

The general outline is given in the current college calendar and the following material will be covered in a series of 40 lectures and 10 laboratories during a 14-week semester.

- **Introduction:**

  The electromagnetic spectrum.
  Interaction of radiation with matter.
  The Boltzmann energy distribution.
  The general layout of a spectrophotometer.
  The laws of spectroscpy

- **Photoelectron and U.V. / Visible spectroscopy**

  Molecular energy levels and the different types of transitions.
  The energies and intensities of the absorbances.
  Applications to main group molecules and transition metal complexes.
  Chromophores and the effects of substituents on their absorption spectra.
  The effects of conjugation, conformation and geometry on the absorption spectra of unsaturated hydrocarbons.
  Woodward's rules.

- **Infra-red spectroscopy**

  Diatomic molecules and the simple harmonic oscillator model.
  Selection rules: fundamentals, overtones and combinations.
  Microwave spectroscopy and the rigid rotor model.
  Rotating / vibrating diatomic molecules.
  Linear and non-linear polyatomic molecules .

- **Mass Spectrometry**

  Types of instrument available and principles of operation.
  Modes of ionization: fragmentation patterns.
  Exact masses, mass of the molecular ions and isotopic ratios.
  Identification of common fragments

- **Introduction to n.m.r. spectroscopy**

  Proton spectra will be used to illustrate the following topics.
  Nuclear structure and spin.
  Effect of external magnetic fields on non-zero spin nuclei.
  Spectrometer design and operation.
  Chemical equivalence and chemical shifts.
  Electronegativity, hybridization and aromaticity.
  Integration for protons
  Magnetic equivalence, coupling mechanisms and coupling constants.
  First and second order spectra.
  Applications to structural determinations for organic molecules.

- **^{13}C n.mr.**

  Isotopic abundance
  Chemical shifts and references
  Multiple scans and assumptions
  Proton coupled and decoupled spectra
  The problems of integration
  Aromatic ring carbons

- **^{19}F n.m.r.**

  Isotopic abundance
  Chemical shifts
  Applications in inorganic chemistry

- **^{31}P n.m.r.**

  Isotopic abundance
  Chemical shifts
  Reference material
  Presentation of spectra
  Biochemical uses

- Multinuclear N.M.R.

  Analysis of n.m.r. spectra from compounds that contain more than two n.m.r. active nuclei

- **Developments**
  Nuclear Overhauser Effect (NOE)
  Fast Fourier methods
  Two dimensional n.m.r.
  Interpretation of COSY Spectra

Learning outcome

At the end of this course a student will have an enhanced ability to:

Introduction:	Describe and explain the production of the various types of electromagnetic radiation. Associate a nuclear, atomic or molecular process with the absorption of radiation a particular frequency. Describe, explain and use the relationships between energy, frequency and wavelength. Describe the Boltzmann distribution of energy and explain its importance to spectroscopic experiments.
General	Give the general layout of a spectrophotometer and describe the choices made for the six major components in each electromagnetic region. Derive and use the laws of absorption spectroscopy.

Types of spectroscopy

Photoelectron	Distinguish between ionizing and non-ionizing radiation. Describe and explain the results of the photoelectric experiment and its extension into photoelectron spectroscopy. Interpret a photoelectron spectrum in terms of the molecular orbitals associated with the molecule and whether the electrons are in bonding or non-bonding orbitals.
U.V. / visible	Describe and explain the processes of absorption and emission in organic and inorganic compounds. Link an absorption at a particular wavelength with the presence of particular structural feature in the compound.
Infra-red	Describe and explain the behavior of diatomic molecules in terms of the simple harmonic oscillator model. Derive the number of modes of vibration for linear and non-linear polyatomic molecules. Interpret an I.R. spectrum in terms of the presence or absence of particular functional groups. Analyze a pure rotational spectra to determine the bond length of the molecules using the rigid rotor model.
Mass Spectrometry	Describe the types of instrument available and the different ways in which the molecular mass is determined. Calculate isotope splitting patterns based the known isotopic ratios found in nature.
N.M.R.	Describe and explain how hydrogen-1, carbon–13, fluorine-19, and phosphorous–31 can be made to absorb radio frequency radiation. Deduce the chemical structures of compounds containing these atoms using tables of chemical shifts, known reference materials and coupled and decoupled spectra.
Problem sets	From a summary of all the spectroscopic data, deduce the full structures of important compounds in organic, inorganic and biochemistry.