CAMOSUN COLLEGE	***School of Arts & Science*** ***CHEMISTRY AND GEOSCIENCE DEPARTMENT*** **CHEM 213- *001*** **Molecular Spectroscopy** **Q2W2007**

COURSE OUTLINE

1. Instructor Information

(a)	Instructor:	Graham Shorthill
(b)	Office Hours:	See the posted times on the office door
(c)	Location:	Fisher 342C
(d)	Phone:	370-3441
(e)	Email:	Shorthg@camosun.bc.ca

2. Intended Learning Outcomes

Upon completion of this course the student will be able to:

1. Describe and explain the production of the various types of electromagnetic radiation and derive and use the laws of absorption spectroscopy.
2. Associate a nuclear, atomic or molecular process with the absorption of radiation of a particular frequency.
3. Describe the Boltzmann distribution of energy and explain its importance in spectroscopic experiments.
4. Explain the results of the photoelectronic experiments and interpret the spectrum in terms of bonding and non-bonding molecular orbitals.
5. Describe and explain the processes of absorption and emission in organic and inorganic compounds and comment on the link between the features of a spectrum and the presence of particular structural features in the compound.
6. Describe and explain the behaviour of diatomic molecules in terms of the simple harmonic oscillator model and derive the number of modes of vibration for linear and non-linear polyatomic molecules.
7. Comment on the features of an IR spectrum in terms of the presence or absence of a particular functional group and analyze the pure rotational spectra to determine the bond length of the molecules using the rigid rotor model.
8. Describe the different ways in which the molecular mass is determined and calculate isotope splitting patterns based on the known isotopic ratios in nature.
9. Describe the absorption of radiation by the hydrogen-1, carbon-13, fluorine-19, and phosphorous-31 nuclei and deduce the chemical structures of compounds containing these nuclei using tables of chemical shifts, known reference materials and coupled and decoupled spectra.

3. Required Materials

Texts and supplies:

“Practical Spectroscopy” by Stendall and Hall
“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 duo tang 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.

4. Course Content and Schedule

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 spectroscopy

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
19F n.m.r.
Isotopic abundance
Chemical shifts
Applications in inorganic chemistry

31P 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

5. Basis of Student Assessment (Weighting)

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%

6. Grading System

Standard Grading System (GPA)

Percentage	Grade	Description	Grade Point Equivalency
95-100	A+		9
90-94	A		8
85-89	A-		7
80-84	B+		6
75-79	B		5
70-74	B-		4
65-69	C+		3
60-64	C		2
50-59	D		1
0-49	F	Minimum level has not been achieved.	0

Temporary Grades

Temporary grades are assigned for specific circumstances and will convert to a final grade according to the grading scheme being used in the course. See Grading Policy at **camosun.ca** or information on conversion to final grades, and for additional information on student record and transcript notations.

Temporary Grade	Description
I	*Incomplete*: A temporary grade assigned when the requirements of a course have not yet been completed due to hardship or extenuating circumstances, such as illness or death in the family.
IP	*In progress*: A temporary grade assigned for courses that are designed to have an anticipated enrollment that extends beyond one term. No more than two IP grades will be assigned for the same course.
CW	*Compulsory Withdrawal:* A temporary grade assigned by a Dean when an instructor, after documenting the prescriptive strategies applied and consulting with peers, deems that a student is unsafe to self or others and must be removed from the lab, practicum, worksite, or field placement.

Temporary grades are assigned for specific circumstances and will convert to a final grade according to the grading scheme being used in the course. See Grading Policy E-1.5 at **camosun.ca** for information on conversion to final grades, and for additional information on student record and transcript notations.

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.

7. Recommended Materials or Services to Assist Students to Succeed Throughout the Course

LEARNING SUPPORT AND SERVICES FOR STUDENTS

There are a variety of services available for students to assist them throughout their learning. This information is available in the College calendar, at Student Services or the College web site at camosun.ca.

STUDENT CONDUCT POLICY

There is a Student Conduct Policy **which includes plagiarism**. It is the student's responsibility to become familiar with the content of this policy. The policy is available in each School Administration Office, at Student Services and on the College web site in the Policy Section.

Summary of Learning Outcomes for CHEM 213

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 spectrum 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.