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| CAMOSUN COLLEGE | ***School of Arts & Science***<br>***CHEMISTRY AND GEOSCIENCE DEPARTMENT***<br>**CHEM 213-01**<br>**Molecular Spectroscopy**<br>**2009W** |

# COURSE OUTLINE

**The Approved Course Description is available on the web @ _____**

Ω *Please note: this outline will be electronically stored for five (5) years only. It is strongly recommended students keep this outline for your records.*

## 1. Instructor Information

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|---|---|---|---|---|
| (a) | Instructor: | Dr. Nasr Khalifa | | |
| (b) | Office Hours: | T, W, Th. 9:30-10:30am, M 9:30-11:30am | | |
| (c) | Location: | F348C | | |
| (d) | Phone: | 250-370-3201 | Alternative Phone: | |
| (e) | Email: | khalifa@camosun.bc.ca | | |
| (f) | Website: | http://khalifa.disted.camosun.bc.ca | | |

## 2. Intended Learning Outcomes

*(No changes are to be made to this section, unless the Approved Course Description has been forwarded through EDCO for approval.)*

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

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|---|---|---|
| (a) | Text | "Organic Structures from Spectra" Fourth Edition, by L. D. Fields, S. Sternhell, and J. R. Kalman (2008) |
| (b) | Lab Manual | "Laboratory Manual and Study Guide" by Graham Shorthill and Nasr Khalifa (2009)<br>*****Both texts are REQUIRED***** |
| (c) | Recommended Texts | "Introduction to Spectroscopy" Fourth Edition by Pavia et al (2009)<br>"Foundations of Spectroscopy" by Duckett and Gilbert, Oxford (2000) |

## 4. Course Content and Schedule

**Detailed Course Outline:**

**1. Introduction:**
-The electromagnetic spectrum
-Interaction of radiation with matter
-The Boltzmann energy distribution
-The general layout of a spectrophotometer
-The laws of spectroscopy

**2. 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

**3. Infra-Red (IR) 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

**4. 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

**5. Introduction to NMR 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

**6. $^{13}$C NMR**
-Isotopic abundance
-Chemical shifts and references
-Multiple scans and assumptions
-Proton coupled and decoupled spectra
-The problems of integration

-Aromatic ring carbons

**7. $^{19}$F NMR**
-Isotopic abundance
-Chemical shifts
-Applications in inorganic chemistry

**8. $^{31}$P NMR**
-Isotopic abundance
-Chemical shifts
-Reference material
-Presentation of spectra
-Biochemical uses

**9. Multinuclear NMR and Developments**
-Analysis of NMR spectra from compounds that contain more than two NMR active nuclei
-Nuclear Overhauser Effect (NOE)
-Fast Fourier methods
-Two dimensional NMR
-Interpretation of COSY Spectra

**Chem213 Laboratory Schedule: (Winter 2009)**
**(subject to change)**

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|---|---|
| Jan. 5: | No Labs. Review problem set |
| Jan. 12: | Exp. 1 |
| Jan. 19: | Exp. 2 |
| Jan. 28: | Exp. 3 |
| Feb. 2: | Exp. 4 |
| Feb. 9 : | **Test #1 (2 hrs)** |
| Feb. 16: | Exp. 5 |
| Feb. 23: | Exp. 6 |
| Mar. 2: | Exp. 7 |
| Mar. 9: | **Test # 2 (2 hrs)** |
| Mar. 16: | Exp. 8 |
| Mar. 23: | Exp. 9/10 |
| Mar. 30: | Exp. 9/10 |
| Apr. 6: | No Labs. Lecture/Review |

*Final exam at the end of the course will cover **all** course material.
*At least a passing grade on lab marks must be achieved in order to write the final exam.
*You must pass both the lecture portion and the lab portion in order to pass the course.
*You must provide your own **safety glasses**. Prescription glasses are OK, but sunglasses are NOT. You must wear these safety glasses at all times while you are in the lab. You will not be allowed to carry out experiments without safety glasses.
*Office hours are posted on the door. You can, however, drop by the office any time. You will not be wasting my time if you come for help. I'm here to help you learn.

## 5. Basis of Student Assessment (Weighting)

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|---|---|---|---|
| (a) | Assignments | Lab Experiments | 25% |
| (b) | Quizzes | | |
| (c) | Exams | Test # 1, Feb. 9 (2 hrs)<br>Test # 2, March 9 (2 hrs)<br>Final Examination (April, 3 hrs) | 15%<br>20%<br>40%<br>---<br>100% |

## 6. Grading System

*(No changes are to be made to this section, unless the Approved Course Description has been forwarded through EDCO for approval.)*

### Standard Grading System (GPA)

| Percentage | Grade | Description | Grade Point Equivalency |
|---|---|---|---|
| 90-100 | A+ | | 9 |
| 85-89 | A | | 8 |
| 80-84 | A- | | 7 |
| 77-79 | B+ | | 6 |
| 73-76 | B | | 5 |
| 70-72 | B- | | 4 |
| 65-69 | C+ | | 3 |
| 60-64 | C | | 2 |
| 50-59 | D | Minimum level of achievement for which credit is granted; a course with a "D" grade cannot be used as a prerequisite. | 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 E-1.5 at **camosun.ca** for 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, due to design may require a further enrollment in the same course. No more than two IP grades will be assigned for the same course. *(For these courses a final grade will be assigned to either the 3rd course attempt or at the point of course completion.)* |
| **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. |

## 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.