Chemistry 2260
Introduction to Spectroscopy
Fall 2019

In Chemistry 2260, we will study how spectroscopy is used to understand the chemical and physical properties of matter on the microscopic scale. In order to describe these principles, a good command of mathematics is essential!

Instructor: Dr. Jennifer van Wijngaarden (she/her)
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Office hours:
M 10:30-11:30, Th 10:30-11:30
…or by appointment W, F (Please email ahead)

Website: Go to the UMLearn site for class announcements, lecture slides, suggested problems.

Texts: The following **e-books** (*available for free through the UManitoba library*) will be used in the course. Links are also provided in UMLearn.

1. ***Physical Chemistry for the Chemical Sciences***, Chang and Thoman, http://bit.ly/ChangThoman
2. ***Basic Atomic and Molecular Spectroscopy***, J. M. Hollas, http://bit.ly/JMHollas

----Please note that each student can save a personal copy of individual chapters on their computer and print them. Students cannot share files or print them for others. Please respect the licensing agreement with the publisher so that we do not lose this privilege of using a free textbook!!!

Grading:

Two Midterms (in class)	**25%**
Final Exam	**55%**
Laboratory	**20%**

****** To pass the course, you must obtain a grade of 50% in the lab and a grade of 50% in the lecture material (term tests, final exam)******

The conversion to final letter grades will be as follows:

A+ >90%	B+ 75-79%	C+ 65-69%	D 50-59%
A 80-89%	B 70-74%	C 60-64%	F <50%

Schedule of Important Dates:

Lab starts	Sept. 10-12
Term test 1	Fri. Oct. 4, in class
Term test 2	Fri. Nov. 1, in class
Final exam	Scheduled by Registrar

Labs:
The lab begins in **350 Parker** during the week of **Sept 10-12** and will be overseen by **Dr. Carl Bartels**. There is a separate UMLearn page for the lab where the lab schedule and manual will be posted. Further information is available during your first lab period.

Please note that the Department is undergoing curriculum changes. Any lab exemptions earned in this course or others in the 2019-2020 academic year will only be honoured for one year and thus must be used in 2020-2021.

Academic Integrity:
There is zero tolerance for academic offences such as cheating and plagiarism in all aspects of this course! All academic misconduct (including lab offences) will be reported to the Department of Chemistry and the Faculty of Science. For more information, read the Faculty of Science penalties and policies on academic misconduct including the section on **improper collaboration**.
http://umanitoba.ca/faculties/science/undergrad/resources/webdisciplinedocuments.html

Homework:
Practice exercises are provided in UMLearn for each chapter. These supplement the lecture material and will help you improve your understanding of core concepts. Final answers (not solutions) will be posted but students are encouraged to ask for help in class or in my office by appointment. Regular practice through homework problems is important preparation for examinations. Assigned problems give you practice with routine calculations (units, solving equations with algebra, etc.) and also challenge you to apply the core concepts in new situations.

Midterm tests:
The two midterm exams account for a total of **25%** of your final grade and will be weighted **8%** and **17%** to favour your higher grade. ***Deferred midterm exams are not available.*** Students missing a midterm as a result of a medical or family emergency can request that the weight of the exam be shifted to the final exam. Appropriate documentation must be provided to the instructor within 48 hours of the missed test and a decision about deferral will be made upon consultation with the Department and Faculty of Science as needed.

Final Exam:
The final exam is **cumulative** and will be based on material presented in the lectures and practiced in the homework and labs. This is scheduled by the Registrar's office during the final exam period in December.

2019 Course Outline:

1. Basis of Spectroscopy (*ca.* 4-5 Lectures)
Overview of quantum chemistry including: Planck's Law, blackbody radiation, wave-particle duality, deBroglie wavelengths, Heisenberg uncertainty principle, Schrödinger equation, operators, wavefunctions, Particle in a 1D box

2. Atomic Spectroscopy (*ca.* 5-6 Lectures)
Interpretation of atomic energy levels and atomic absorption/emission spectra including: Bohr model, Rydberg model, QM solution of H atom, multi-electron atoms, atomic term symbols, Hund's rules, photoelectron spectroscopy

3. Vibrational Spectroscopy (*ca.* 5-6 Lectures)
Discussion of molecular vibration and interpretation of infrared and Raman spectra of linear and nonlinear molecules including: Hooke's law, QM solution of vibration (harmonic oscillator), effect of anharmonicity, selection rules

4. Rotational Spectroscopy (*ca.* 4-5 Lectures)
Understanding molecular rotation and interpretation of microwave and infrared spectra of various tops including: classical description of rotation, QM solution of molecular rotation (linear rigid rotor), Boltzmann populations and degeneracies, effect of molecular non-rigidity and multiple moments of inertia, rovibrational spectra (diatomic)

5. Electronic Spectroscopy (*ca.* 6-7 Lectures)
Relating electronic structure of molecules to ultraviolet/visible and X-ray spectra including: discussion of molecular orbitals and energy levels starting with H_2^+ and extending to C_{60}, vibrational (and rotational) structure of electronic spectra, Franck-Condon principle, photoelectron spectroscopy, Koopman's theorem

6. Nuclear Magnetic Resonance Spectroscopy (*ca.* 4-5 Lectures)
Understanding the origin of patterns observed from probing nuclei in magnetic fields including: physical basis (angular momentum, magnetic moments, nuclei in magnetic fields) of NMR, chemical shifts and their interpretation, spin-spin coupling patterns