The University *of* Western Ontario
Department of Chemistry

Chemistry 3374A
QUANTUM CHEMISTRY AND SPECTROSCOPY

Fall 2021

Course Information

Instructor: Prof. Viktor N. Staroverov
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Lectures and Tutorials: Monday, Wednesday, Friday, 10:30 AM – 11:30 AM, NCB 117
Thursday, 11:30 AM - 12:30 PM, NS 7

Office hours: by appointment

Course web site: `https://owl.uwo.ca/portal`

Prerequisite: Chemistry 2384B (Antirequisite: Physics 3200A/B)

Unless you have either the requisites for this course or written special permission from your Dean to enroll in it, you may be removed from this course and it will be deleted from your record. This decision may not be appealed. You will receive no adjustment to your fees in the event that you are dropped from a course for failing to have the necessary prerequisites.

Brief Description: Basic concepts of quantum mechanics are introduced and applied to a variety of problems in chemistry and spectroscopy. Topics include quantum behavior of microscopic particles, principles of vibrational, rotational, and electronic spectroscopy, and the foundations of the quantum theory of chemical bonding.

Optional text: P. Atkins, J. de Paula, and R. Friedman, *Physical Chemistry: Quanta, Matter, and Change* (2nd ed., W. H. Freeman & Co., NY, 2014) or *Quanta, Matter, and Change: A Molecular Approach to Physical Chemistry* (1st ed., W. H. Freeman & Co., NY, 2009). The course covers Focuses 1–5 of the 2nd edition or, equivalently, Chapters 1–4 of the 1st edition, as well as all sections titled "Mathematical background". The 1st edition is on 1-day reserve at the Taylor Library.

Midterm tests: *Test 1*: Wednesday, October 13, in class. *Test 2*: Wednesday, November 17, in class. Format: written answers to questions and problems.

Final exam: Cumulative, 3 hours, time and place TBA.

Assignments and quizzes: Five assignments will be posted throughout the course (see the schedule on p. 2). The assignments themselves will not be marked. However, on the due date there will be a **quiz** asking you to solve a problem that is similar to one of the problems of the assignment. During the quiz, you are allowed to use *only* your written solutions prepared at home and not any other materials. The quizzes will be marked. You are required to write at least 4 out of the total of 5 quizzes. If and only if you write all of the 5 quizzes, you will earn a **bonus**: the quiz for which you received the lowest score will not be counted toward your course grade.

Evaluation: The final course grade will be a weighted average calculated as follows: Quizzes = 20% (four best marks, 5% each), Midterm Test 1 = 20%, Midterm Test 2 = 20%, Final Exam = 40%.

Assignment/Quiz Schedule

#	*Assignment posted (Thursday)*	*Quiz date (Thursday)*
1	September 16	September 23
2	September 30	October 7
3	October 21	October 28
4	October 28*	November 11
5	November 25	December 2

* Before the Fall Reading Week of November 1–7

Topics

1. *Wave-particle duality of microscopic matter.* Inability of classical mechanics to describe the structure of atoms and molecules. Quanta of light and energy. Wave-particle duality. De Broglie waves and their experimental observation.
2. *The Schrödinger equation.* Differential equations. The Schrödinger equation for a microscopic particle. Complex numbers and functions. Probability and probability density. Wave functions and their physical interpretation. Operators, eigenfunctions and eigenvalues. Hamiltonians.
3. *Translational motion of free and confined electrons.* A free particle. A particle in a potential box in one, two, and three dimensions. Chemical applications of the particle-in-a-box model. Rectangular-box model of the chemical bond. Quantum tunneling through a potential barrier.
4. *Mathematical formalism of quantum chemistry.* Operators of physical observables. The postulates of quantum mechanics. Superposition of wave functions. Individual measurements and expectation values. Commuting and non-commuting operators. The Heisenberg uncertainty principle. Transition dipole moment. Intensity of spectroscopic transitions. Selection rules.
5. *Quantum-mechanical description of vibrational motion*. The harmonic oscillator. The Schrödinger equation for a harmonic oscillator. Connection between harmonic oscillators and vibrations of diatomic molecules. Selection rules for vibrational transitions.
6. *Quantum-mechanical description of rotational motion*. The Schrödinger equation for a particle in a ring. Rotation in two and three dimensions. Angular momentum and its quantization. Spherical harmonics. The rigid rotor and rotational spectroscopy of diatomic molecules.
7. *The structure and spectra of hydrogenic atoms.* The Schrödinger equation for one-electron atoms and ions. Energy levels, electronic wavefunctions, and probability densities for hydrogenic atoms. Atomic orbitals and quantum numbers. The spin.
8. *Many-electron atoms.* The orbital approximation for many-electron wave functions. Self-consistent field. The Pauli exclusion principle. The *Aufbau* principle and the periodic table.

Learning Outcomes

1. Recognizing that quantum mechanics is the theoretical basis for all of chemistry and spectroscopy.
2. Understanding of key concepts of quantum mechanics: wave-particle duality, operators, wavefunctions, eigenstates, uncertainty principle, expectation values, orbitals, orbital energies, etc.
3. Ability to set up, solve, and interpret solutions to the Schrödinger equation for chemically relevant model systems: particle in a box, tunneling, harmonic oscillator, rigid rotor, one-electron atoms.
4. Practical skills in applying the results of quantum mechanics to simple problems in vibrational, rotational, and electronic spectroscopy of atoms and molecules.

Policies

Minimum requirements. To pass this course, you must attempt at least two (2) of the five quizzes, at least one of the two midterm tests, the final exam, and get an overall course grade of at least 50%. These requirements must be met even taking into account the approved academic accommodations and/or absences including self-reported absences (SRA).

Missed quizzes. There are no make-up quizzes. At most one quiz may be missed without penalty or need to provide any reason or documentation whatsoever. A student who misses more than one quiz will receive a mark of zero for all quizzes after the first unless academic accommodation is granted through the Dean's Office or the SRA Form. Note that missing more than 3 quizzes, whether excused or not, will make it impossible to satisfy the minimum requirements to pass the course.

Missed tests and exams. If you are unable to write a midterm test, you must request an academic consideration as explained in `https://www.uwo.ca/sci/counselling/index.html` → PROCEDURES → `Academic Consideration for Absences`. It is the student's responsibility to make alternative arrangements with their instructor once the accommodation has been approved and the instructor has been informed. If a student misses one midterm and receives academic accommodation, half of the weight of the missed midterm will be transferred to the other midterm and the second half to the final exam (i.e., the other midterm and final will become worth 30% and 50%, respectively). A combined make-up midterm test will be offered only to students who miss each of the two scheduled midterms and receive academic accommodations for both.

Class attendance. Information missed during unexcused lecture and tutorial absences will not be considered as grounds for academic appeals.

Use of electronic devices. As a courtesy to your fellow classmates, please leave mobile devices at home or switch them to silent mode before lectures begin. If you use a laptop to take notes, please sit near the back of the classroom in order to minimize disruption to other students. During tests and exams, only basic electronic calculators are allowed; all other devices (cell phones, tablets, cameras, or iPod, etc.) are strictly prohibited. Those devices must be left either at home or with the student's bag/jacket at the front of the room and must not be at the test/exam desk or in the individual's pocket. Any student found with one of these prohibited devices will receive a grade of zero on the test or exam. The Department of Chemistry is not responsible for stolen/lost or broken devices.

Academic offences. All work submitted for a grade in this course must be your personal work. Use of answers obtained externally is prohibited. Plagiarism and cheating offences will be reported to the Department Chair for consideration of disciplinary action as noted in Western's "Scholastic Discipline for Undergraduate Students".

Accessibility. Students with disabilities work with Accessible Education (formerly SSD) which provides recommendations for accommodation based on medical documentation or psychological and cognitive testing. For more information, see "Western University Policy on Academic Accommodation for Students with Disabilities".

Support Services. Counselors at the Student Development Centre (`http://www.sdc.uwo.ca`) can help you improve your learning skills. They offer presentations on strategies for improving time management, exam preparation/writing, textbook reading, and more. Individual support is offered in the drop-in Learning Help Centre and through individual counselling. Students who are in emotional/mental distress should refer to Mental Health at Western (`http://www.health.uwo.ca/mental_health`). Additional student-run support services are offered by the USC (`http://westernusc.ca/services`).