**CHEM 3010 M, 3 credits: Physical Chemistry**
**Quantum Chemistry and Spectroscopy**
**Course Outline, Winter 2019**

prerequisite: CHEM 2011

Instructor: René Fournier, Petrie 303, renef@yorku.ca, phone ext. 30687

Required Text: *Physical Chemistry (PC), by Thomas Engel and Philip Reid (Pearson Prentice Hall) 3rd edition (2013)*, ISBN-13: 978-1-292-02224-8. PC is also available as two "half-books": *Quantum Chemistry and Spectroscopy* (QCS) ISBN-13: 978-0321766199, and *Thermodynamics, Statistical Thermodynamics, & Kinetics* (TSTK) ISBN-13: 978-0321766182. The half that you need for CHEM 3010 is QCS: as far as CHEM 3010 is concerned QCS has all the material from PC that we need and it is identical to PC. The required book for CHEM 2011 is PC, or the other half, TSTK. So, if you don't have PC but you have TSTK, you can buy the other half (QCS) and you will have everything.

Lectures: LSB 105, MWF 10:30–11:20
Tutorials: LSB 105, Friday 13:30–14:20
Moodle: I will post lecture notes, assignments and announcements from time to time.
Office hours: Petrie 303, MW 12:00-13:00, except Jan 21 and 28

Information about York's policies on academic honesty, accomodations for students with disabilities, religious observance, etc., is available at
http://www.yorku.ca/secretariat/policies and at
http://secretariat.info.yorku.ca/senate/academic-standards-curriculum-and-pedagogy-committee/
under "Course Information for Students".

Topics covered: quantum mechanics, the particle in a box, vibrational and rotational spectroscopy of diatomic molecules, the hydrogen atom, many-electron atoms, $H_2$ and the chemical bond, electronic spectroscopy, the Boltzmann distribution. This corresponds roughly to chapters 12 to 23 and chapter 25 of PC; or chapters 1 to 10 and chapter 14 of QCS.

## Evaluation

Three tests: 60% (20% each)
Final exam: 40%

The three **tests** will be 50 minutes long and worth 20 marks each, and will be held during regular class time. If you miss any test, your marks will be moved to the final exam. The **final exam** in April will be 3 hours long.

## Organization of the course

You may wish to take notes during class. I don't advise you to write down everything I show. It is more important to listen to what I say, try to follow "in real time", and ask questions, than to write down everything. My lecture notes, and yours, are only summaries and comments about the book's content, they are not a substitute for it. I will post my lecture notes on Moodle at the end of every week. *These lecture notes are in condensed form, they do not include everything I show in class.*

I will assign problems from time to time. These assignments will not be marked, but they are very important. They will be an essential element for you to study in preparation for the tests and exam.

As a rule, you should count roughly two hours of study and practice (e.g., assignments) for every lecture hour.

<u>Important dates</u>

- Wednesday January 30: test #1
- Monday February 18: Family Day, University is closed
- Monday February 18 to Friday February 22: Reading Week, no class
- Monday March 4: test #2
- Friday March 8: last date to drop a course without receiving a grade
- Wednesday April 3: test #3
- Wednesday April 3: last day of class and for late withdrawal ("W" on transcript)

**CHEM 3010, Quantum Chemistry and Spectroscopy**
**Learning Outcomes**

By the end of the term you should be able to ...

1. Explain the differences between classical mechanics (CM) and quantum mechanics (QM).
2. Describe key experiments that led to QM: photoelectric effect, electron diffraction, the H atom spectrum, blackbody radiation.
3. Calculate the photon energy, wavelength, and frequency associated with transitions between energy levels in atoms and molecules.
4. Compare the Bohr and Schrödinger descriptions of the H atom.
5. Identify situations where QM is needed using concepts like the DeBroglie wavelength, the physical dimensions of a system, energy level separations and temperature.
6. Explain what are wave-particle duality and the Heisenberg uncertainty principle.
7. Carry out simple calculations with complex numbers.
8. Give a general discussion of the Schrödinger equation, its different terms, how it is solved, and what its solutions mean.
9. Explain the differences between the time-dependent and time-independent Schrödinger equations.
10. Carry out simple calculations with eigenvalue equations.
11. Discuss the physical meaning of eigenvalues and eigenfunctions associated with QM operators, in particular, how they relate to measurements.
12. Explain the meaning of "normalized", "orthogonal", "orthonormal" and "complete set" and their relevance for physical chemistry.
13. Discuss the postulates of QM.
14. Carry out simple calculations using the eigenvalues and/or eigenfunctions of model systems: the free particle (FP), the particle in a box (PIB), the particle on a ring (POR, also called rigid rotor), the particle on a sphere (POS), and the harmonic oscillator (HO)
15. Discuss the correspondence principle using the PIB.
16. Explain the technique of separation of variables using the 3-dimensional PIB.
17. Use the PIB model to describe qualitative aspects of atoms, chemical bonds, $\pi$ conjugated systems, metals, and insulators.
18. Evaluate commutators of pairs of operators and explain their relevance for QM.
19. Explain the Stern-Gerlach experiment and discuss electron spin.

20. Describe qualitatively the different degrees of freedom in molecules: electronic, vibrational, rotational and translational.

21. Describe the harmonic oscillator (HO), its treatment in CM and QM, and key results about vibrations of diatomic molecules.

22. Describe the rigid rotor (or particle in a ring, POR), its treatment in QM, and key results about molecular rotations.

23. Explain how separation of variables is used to describe the motion of nuclei in QM as a product of a translational wavefunction, a rotational wavefunction, and a vibrational wavefunction.

24. Describe spherical harmonics and explain their role in the wavefunctions associated with molecular rotations and in orbitals (electronic wavefunctions).

25. Carry out simple calculations involving eigenfunctions, eigenvalues or quantum numbers of the POR, POS and HO models.

26. Discuss rotational and vibrational spectra in general and the relevant parts of the electromagnetic spectrum (microwave, infrared).

27. Discuss rotational and vibrational spectra in relation to energy levels and quantum numbers in the POR, POS and HO models.

28. Use selection rules, energy level expressions, and Planck's relation in simple spectroscopic calculations.

29. Use the Boltzmann relation for the population of energy levels in typical situations of physical chemistry.

30. Describe the H atom, the relevant Schrödinger equation, and orbitals obtained from it.

31. Discuss the orbital approximation, and orbitals, for many-electron atoms.

32. Discuss the symmetry of wavefunctions under exchange of identical particles, spin, the Pauli principle, and how they lead to singlet and triplet states.

33. Use the variational principle in simple situations.

34. Explain the SCF method and Slater determinants for many-electron atoms.

35. Discuss the electronic configurations of atoms.

36. Define and use ionization energy, electron affinity, Mulliken electronegativity, and Pearson-Parr hardness.