

## CHEM 360: Quantum Chemistry (Fall 2023)

- Contact:** Professor Allan East, Room RI312. Office Hours: 13h30-14h30 MTWF, or by appointment. Don't be shy - I want to help! E-mail: allan.east@uregina.ca.
- Text:** *Physical Chemistry*, P. Atkins and coauthor(s), 11th ed. (ch. 7,8,9,11). The 10th edition is fine too (ch. 7,8,9,10,12).
- Grading Scheme:** Problem Sets 20%, Test 1 20%, Test 2 20%, Final Exam 40%.  
Final Exam: Dec. 21, 09h00 to 12h00
- Problem Sets:** Roughly 8 week-long ones, HAND-WRITTEN ONLY on lined paper and stapled together before handing in, in class or under my door. Show your work; in the math problems, show each step you can't do in your head, and mention when you are using an outside source to solve an integral. Remember: the point of assignments is to get practice for tests and exams, so I still recommend doing the math step-by-step on paper with a calculator.  
  
YOU MUST AVOID PLAGIARISM or you will lose credit. Plagiarism is the act of COPYING: either a sequence of steps exactly or the answer itself, from another source (classmate or artificial intelligence!) tasked with the same question, and handing it in for credit. If you are only checking a source for help on how to START a problem, or for COMPARING to see if you are "on the right track" or not, that is okay with me. If you are copying things like a standard integral table result or an atomic mass, that is okay (and expected), but cite your source for any used integral result. My tips for how to work with a friend are:
  - try each problem at the same time but without consulting,
  - if one is stuck, consult verbally first,
  - IF you show your work to another student, DON'T LET IT LEAVE YOUR HANDS. THIS INCLUDES SENDING PHOTOS OF IT TO OTHER STUDENTS. This will tempt even the best of friends into plagiarism, and you both would be penalized.
- Lectures:** in classroom LB206, MTTh 09h30. Bring a notebook to take notes - almost all lectures are planned as inkboard lectures, and since the tests are hand-written, you need to practice copying and writing down the math examples (many integrals and derivatives).
- Course Outline:** (Bracketed numbers match the 11th edition of the Atkins text)

<u>I. Quantum Mechanics</u> (7A) Origins of quantum mechanics (7B) Wavefunctions (7C) Operators, expectation values (7D) Particle in a Box (Translations) (7E) Harmonic Oscillator (Vibrations) (7F) Rigid Rotor (Rotations) (not in text): Perturbation theory	<u>III. Molecules</u> (9B) Hamiltonians, LCAO-MOs, E+ and E- (9CD) Diatomic VOMELDS (valence-orbital mixing energy-level diagrams) (not in text) Polyatomics VOMELDs, nucleophiles, resonance (9E.3) Computational Chemistry: introduction (not in text) Rovibronic energy levels (11B) Rotational (microwave) transitions (11C) Diatomic vibrational (infrared) transitions (11D) Polyatomic vibrational (infrared) transitions
<u>II. Atoms</u> (8A) One electron (8B) Many electrons (8C) Spectra and term symbols	