This course introduces the biochemistry major to quantum chemistry: atomic and molecular structure and spectroscopy. Applications of these in biochemical situations will be explored. The section on statistical thermodynamics will apply the principles of quantum chemistry toward a microscopic view of thermodynamics.

**TOPIC** | **CHAPTER**
--- | ---
Quantum Theory | 7
Atomic Structure | 8

**EXAM I**: February 20

Molecular Structure | 9
Symmetry | 10
Molecular Spectroscopy | 11, S:5

**EXAM II**: April 10

Magnetic Resonance Spectroscopy | 12
Statistical Mechanics | 13
Electric and Magnetic Properties | 14

**FINAL EXAM**: May ?? (5:15-7:15)
GRADING POLICY

Each semester exam is worth 300 points; the final is worth 400 points. All in-class exams must be done with non-communicating devices (pencil, pen, slide rule, abacus, noncommunicating calculator). Use of a communicating calculator on an in-class exam will result in a score of 0 on that assignment. The instructor reserves the right to further limit the use of calculators on in-class exams.

Students enrolled in CH 561 will also be required to write a 7-10 page paper describing a development in molecular spectroscopy, quantum mechanics, or statistical mechanics. The paper will be due May 8.

Homework will be assigned, but not collected.

Students with Disabilities

Reasonable academic accommodations may be provided to students who submit relevant and current documentation of their disability. Students are encouraged to contact the Center for Teaching and Learning Excellence (CTLE) at disabilityservices@scranton.edu or (570) 941-4038 if they have or think they may have a disability and wish to determine eligibility for any accommodations. For more information, please visit http://www.scranton.edu/disabilities.

Writing Center Services

The Writing Center focuses on helping students become better writers. Consultants will work one-on-one with students to discuss students’ work and provide feedback at any stage of the writing process. Scheduling appointments early in the writing progress is encouraged. To meet with a writing consultant, call (570) 941-6147 to schedule an appointment, or send an email with your available meeting times, the course for which you need assistance, and your phone number to: writing-center@scranton.edu.

The Writing Center does offer online appointments for our distance learning students. Please contact Amye Archer at amye.archer@scranton.edu for more information.

Academic honesty:

The first time that a student is caught plagiarizing or using fabricated data in a report, he or she will receive a grade of zero points for that assignment. For further consequences of violating academic ethics please refer to the University of Scranton Student Handbook.
ASSIGNMENTS

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The SLO Track

In completing this course students should be able to:

1. calculate an observable property of a quantum system using operators and wavefunctions.
2. determine the energy of the ground state of one-electron atom or ion.
3. predict the ground state of an atom or ion.
4. build a molecule using Gaussview or Avogadro.
5. predict the structure and properties of a molecule using Gaussian.
6. determine the point group of a molecule.
7. predict the electronic ground state of a diatomic molecule.
8. predict spectroscopic parameters from structure calculations and vice-versa.
9. calculate thermodynamic properties of a molecule from spectroscopic and structural information.
10. estimate the dipole moment of a molecule using bond dipoles.
11. estimate the effect of hydrogen bonding in IR, UV-visible, and fluorescence spectroscopy.