

CHEM 361 BIOPHYSICAL CHEMISTRY II
CHEM 561 INTRODUCTION TO QUANTUM CHEMISTRY

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Texts: “Physical Chemistry” Twelfth Edition, Volume 2, P.W. Atkins, J. de Paula, J. Keeler
“Biochemical Calculations” Second Edition, I. Segel.

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 17	
Molecular Structure	9
Symmetry	10
Molecular Spectroscopy	11, S:5
Magnetic Resonance Spectroscopy	12
EXAM II : April 7	
Statistical Mechanics	13
Electric and Magnetic Properties	notes
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 7.

Homework will be assigned, but not collected.

Students with Disabilities

Students with disabilities may be eligible for reasonable academic and non-academic accommodations. Students are required to submit relevant and current documentation of their disability. Students are encouraged to contact the Office of Student Support and Success 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 academic accommodations. For non-academic accommodations, students should contact the Office of Equity and Diversity at non-academic-accom@scranton.edu or (570) 941-6645. Students can access accommodate by clicking [here](#).

Writing Center Services

The Writing Center is a resource designed to help students at all academic levels become better writers. It is a safe space where students from any discipline can receive one-on-one feedback on written assignments from well-trained peer consultants who support students in any stage of the writing process. Students can make an appointment through the my.scranton portal: [my.scranton.edu >OSSS Card >Writing Center Scheduler](#).

For more information, please contact writing-center@scranton.edu. For quick tips, user-friendly guides, and other writing resources, check out our blog at <https://sites.scranton.edu/writingcenter>.

<https://www.scranton.edu/academics/ctle/writing/index.shtml> .

Academic honesty:

The first time that a student is caught cheating on an exam or is caught plagiarizing 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.

<https://www.scranton.edu/academics/cte/acad-integ/acad-code-honesty.shtml>

ASSIGNMENTS

Chapter	Exercises/Problems
7	E: A.7-17, B.3-8, C. 9, D. 12, 19-21, E. 7-10, F. 13-16 P: B.7, C.1, D.1,2, E.3,4, F.4
8	E: A. 9-14, B. 7-9, C. 10-14/ P: A. 4, C. 1,2
9	E: B. 4, C. 6-13, D. 4-9, E. 7-11/P: B. 1, C. 4, E. 9
10	E: A. 9-13/ P: A. 1-4
11	E: A. 9-11, B. 13, 16, 17, C. 6-11, D. 8-12, E. 4-6, F. 7-11, P: B. 6, C. 10, 11, E. 1, F. 1-3
12	E: A. 9-12, B. 10-14, D. 6-11
13	E: A.10-12, B. 9-13, E. 8-10, 14, 15, 17, 18 F. 5, 6
S 5	1-4

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.

My Reporting Obligations as a Required Reporter

As a faculty member, I am deeply invested in the well-being of each student I teach. I am here to assist you with your work in this course. Additionally, if you come to me with other non-course-related concerns, I will do my best to help. It is important for you to know that all faculty members are required to report incidents of sexual harassment or sexual misconduct involving students. This means that I cannot keep information about sexual harassment or discrimination, sexual assault, sexual exploitation, intimate partner violence or stalking confidential if you share that information with me. I will keep the information as private as I can but am required to bring it to the attention of the University's Title IX Coordinator, Elizabeth M. Garcia, or Deputy Title IX Coordinator, Diana Collins Gilmore, who, in conversation with you, will explain available support, resources, and options. I will not report anything to anybody without first letting you know and discussing choices as to how to proceed. The University's Counseling Center (570-941-7620) is available to you as a confidential resource; counselors (in the counseling center) do not have an obligation to report to the Title IX Coordinator.

Non-Discrimination Statement

The University is committed to providing an educational, residential, and working environment that is free from harassment and discrimination. Members of the University community, applicants for employment or admissions, guests, and visitors have the right to be free from harassment or discrimination based on race, color, creed, religion, ancestry, gender, sex, pregnancy and related conditions, sexual orientation, gender identity or expression, age, disability, genetic information, national origin, ethnicity, family responsibilities, marital status, veteran or military status, citizenship status, or any other status protected by applicable law.

Students who believe they have been subject to harassment or discrimination based on any of the above class of characteristics, or experience sexual harassment, sexual misconduct or gender discrimination should contact Elizabeth M. Garcia, Title IX Coordinator, (570) 941-6645 elizabeth.garcia2@scranton.edu, or Deputy Title IX Coordinators Diana Collins Gilmore (570) 941-6645 diana.collinsgilmore@scranton.edu. The United States Department of Education's Office for Civil Rights (OCR) enforces Title IX. Information regarding OCR may be found at www.ed.gov/about/offices/list/ocr/index.html.