Physical Chemistry I: Quantum Chemistry
Syllabus for Fall 2025 Term

GENERAL INFORMATION

RUTGERS CATALOG DESCRIPTION

50:160:345-346 Physical Chemistry I,II (3,3): Thermodynamics with chemical applications, kinetics, quantum mechanics, statistical mechanics, transport, and structure. **Prerequisites for 50:160:345:** 50:160:116 & 50:160:126 (Chemical Principles II + Lab), 50:640:221 (Calculus III), 50:750:131-134 (Elements of Physics I & II + Labs). **Prerequisite for 50:160:346:** 50:160:345.

Course Format: Lectures

Instructor: **Dr. Guillaume Lamoureux**
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Office Hours: By appointment
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Lectures: Tuesdays and Thursdays from 9:35 to 10:55
Location: CNS-213

Textbook: **Atkins, De Paula & Keeler, *Atkins' Physical Chemistry*, 12th Edition.** Although the material for this course is contained in Volume 2, which can be bought separately, it is best to buy the full textbook if you plan on taking Physical Chemistry II (50:160:346) as well. If you are considering using an earlier edition of the book, please confirm with the instructor.

Review Material: In preparation for the course, please review the following chapters from **Cutnell & Johnson, *Physics*, 12th Edition** (or the equivalent chapters from any other calculus-based Introductory Physics textbook):
- Newton's laws of motion (Chapter 4)
- Rotational motion (Chapters 8 and 9)
- Harmonic motion (Chapter 10)
- Waves (Chapters 16 & 17)
- Electrostatics (Chapters 18 & 19)
- Magnetism (Chapter 21)
- Electromagnetic waves (Chapter 24)

TOPICS

The course introduces students to the concepts of quantum mechanics and the electronic structure of atoms and molecules. The following topics will be covered: (1) introduction to quantum theory, (2) quantum theory of motion, (3) atomic structure and spectra, (4) molecular structure, (5) rotational, vibrational and electronic spectroscopy.

COURSE GRADE

The final grade for the course is composed as follows: **20% for in-class tests, 20% for the first midterm exam, 20% for the second midterm exam, and 40% for the final exam**. The minimum passing grade for the course is 60%.

COURSE MATERIAL

All material for the course (except the textbook) will be posted on Canvas (https://canvas.rutgers.edu). Please consult the website regularly and set your notifications so that you get informed of any update.

BEFORE EACH LECTURE
You are expected to read the appropriate sections of the textbook ahead of time and to have identified the concepts you are not clear about. To make time for tests and problems in class, some of the lectures will be pre-recorded and posted on Canvas. You are expected to watch them ahead of time and take notes the same way you would take notes in class.

IN-CLASS TESTS
There will be 6 tests during the term, to be completed in class after similar problems will have been discussed by the instructor. The tests will not be announced, so you may miss one if you do not attend all lectures. To accommodate the occasional absence, only your best 4 tests out of the 6 will be used to calculate your grade. (Each one will be worth 5% of the final grade) These tests are meant to assess your ability at transposing a given logical procedure to a slightly different situation. Always bring your calculator in class.

EXAMINATIONS
The midterm exams will be held on **October 14** and **November 13**. The final exam date is set by the Office of Scheduling and will be announced later during the term. If you are absent from a midterm exam, you must produce a note appropriately signed (e.g., by a doctor or an employer) on letterhead paper. This note must be delivered no later than one week after the exam date. If the absence is not valid, you will receive a mark of zero for the missed exam. If it is valid, the two other exams will be worth 70% of the final grade and all of your 6 tests will be counted (for 30% of the final grade).

ACADEMIC INTEGRITY
Rutgers University takes academic dishonesty very seriously. By enrolling in this course, you assume responsibility for familiarizing yourself with the Academic Integrity Policy and the possible penalties (including suspension and expulsion) for violating the policy. As per the policy, all suspected violations will be reported to the Office of Community Standards. Academic dishonesty includes (but is not limited to): cheating, plagiarism, aiding others in committing a violation or allowing others to use your work, failure to cite sources correctly, fabrication, using another person's ideas or words without attribution, re-using a previous assignment, unauthorized collaboration, sabotaging another student's work. If in doubt, please consult the instructor. Please review the Academic Integrity Policy at http://academicintegrity.rutgers.edu.

STUDENTS WITH DISABILITIES
Rutgers University welcomes students with disabilities into all of the University's educational programs. In order to receive consideration for reasonable accommodations, a student with a disability must contact the appropriate disability services office at the campus where you are officially enrolled, participate in an intake interview, and provide documentation: https://ods.rutgers.edu/students/documentation-guidelines. If the documentation supports your request for reasonable accommodations, your campus's disability services office will provide you with a Letter of Accommodations. Please share this letter with your instructors and discuss the accommodations with them as early in your courses as possible. To begin this process, please complete the registration form at https://webapps.rutgers.edu/student-ods/forms/registration.

PRACTICE PROBLEMS
A list of suggested practice problems from the book will be provided with each section. It is your responsibility to use these problems to practice in applying the course material.

SOME ADVICE
Note taking: Taking handwritten notes during the lectures (either in class or pre-recorded) is an important exercise in itself: It develops your mathematical skills and your capacity at synthesizing what is being said. You will not absorb the material nearly as well if you just watch the instructor go through it. **Reading/studying:** Read the textbook on your own first but make sure you eventually

meet with your classmates to revise the important concepts and check your understanding against theirs. When reading the textbook, keep track of all questions you have and use classroom time to ask them. **Practice problems:** It is very unlikely that you will be successful in this course if you do not practice the material. Make the most of the time you spend on each problem by asking yourself: What are the concepts or skills being learned? What other questions could arise from the situation described? Could the problem be formulated in more general (or more specific) terms? For quantitative questions, aim to develop your knowledge and your intuition to the point where you can guess what the answer is (within a couple of orders of magnitude) before even attempting any calculation.

CALENDAR OF LECTURES

Please note that this calendar may change as the semester proceeds. The chapter numbers refer to the 12th edition of the textbook.

Date	Topics	Reading
Sep. 2	Introduction, The origins of quantum mechanics	7A
Sep. 4	The origins of quantum mechanics (cont'd)	
Sep. 9	Wavefunctions	7B
Sep. 11	Operators and observables	7C
Sep. 16	Operators and observables (cont'd)	
Sep. 18	The quantum theory of motion	7D
Sep. 23	The quantum theory of motion (cont'd)	7E
Sep. 25	The quantum theory of motion (cont'd)	7F
Sep. 30	The quantum theory of motion (cont'd)	
Oct. 2	Hydrogenic atoms	8A
Oct. 7	Hydrogenic atoms (cont'd)	
Oct. 9	Many-electron atoms	8B
Oct. 14	**Midterm Exam #1 (covers Chapter 7 and Topic 8A)**	
Oct. 16	Atomic spectra	8C
Oct. 21	Atomic spectra (cont'd)	
Oct. 23	Valence-bond theory	9A
Oct. 28	Molecular orbital theory	9B
Oct. 30	Molecular orbital theory (cont'd)	9C
Nov. 4	Molecular orbital theory (cont'd)	9D
Nov. 6	Molecular orbital theory (cont'd)	
Nov. 11	Molecular symmetry	10A
Nov. 13	**Midterm Exam #2 (covers Chapters 8 and 9)**	
Nov. 18	General features of molecular spectroscopy	11A
Nov. 20	Rotational and vibrational spectroscopy	11B & 11C
Nov. 25	Rotational and vibrational spectroscopy (cont'd)	11D
Nov. 27	NO LECTURE	
Dec. 2	Electronic spectra, Decay of excited states	11F & 11G
Dec. 4	Electronic spectra, Decay of excited states (cont'd)	
Dec. 9	Review	
TBA	**Final Exam (cumulative)**	