

Physical Chemistry I: Quantum Chemistry

Syllabus for Fall 2022 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**

Office: Joint Health Sciences Center 216C

Office Hours: Immediately after the Tuesday lectures

Any other time: By appointment

Email: guillaume.lamoureux@rutgers.edu

Website: <http://lamoureuxlab.org/teaching.html>

Lectures: Tuesdays and Thursdays from 9:35 to 10:55

Location: CNS-213

Textbook: **Atkins, De Paula & Keeler, *Atkins' Physical Chemistry*, 11th Edition.**

(The textbook is available for sale at <https://universitydistrict.bncollege.com> and for short-term loans at the Robeson Library Reserve. If you are considering using an earlier edition of the book, please check with the instructor first.)

Review Material: In preparation for the course, please review the following chapters from **Cutnell & Johnson, *Physics*, 10th Edition** (or the equivalent chapters from any other algebra-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)

COURSE TOPICS

The course introduces students to the concepts of quantum mechanics and the electronic structure of atoms and molecules. After a review of classical physics, 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, (6) magnetic resonance.

COURSE GRADE

The final grade for the course is composed as follows: **18% for the assignments, 21% for the first midterm exam, 21% 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 updates.

BEFORE EACH LECTURE

Students are expected to read the appropriate sections of the textbook ahead of time.

EXAMINATIONS

The midterm exams will be held on **October 13** and **November 15**. The final exam date is set by the Office of Scheduling and will be announced later during the term. If a student is absent from a midterm exam, he/she must produce a note appropriately signed (e.g., by a doctor or an employer) on letterhead paper. This note must be delivered to the instructor no later than one week after the exam date. If the absence is not valid, the student will receive a mark of zero for the missed exam. If it is valid, the two other exams will be worth 82% 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>.

GRADED ASSIGNMENTS

There will be 3 graded homework assignments during the term. Each assignment will be due one week after it is handed out. Late assignments will be deducted **10% per day late**. Any assignment handed in more than 5 days late will be given a grade of zero. If you need more time to complete an assignment, ask the instructor for an extension before the deadline.

PRACTICE PROBLEMS

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

SOME ADVICE

Note-taking: Take copious notes and keep expanding them as you study and practice the material. Note-taking during class and when reading the textbook is an important exercise in itself. Given the nature of the material (equations and graphs), notes are best taken using either a notebook or loose sheets of paper (numbered, kept in a folder). **Reading/studying:** It is best to read the material on your own first but make sure you eventually meet with your classmates to revise the important con-

cepts and compare your understanding with theirs. The best way to understand something is to try explaining it to somebody else. When you read the textbook, keep track of any question you have. **Practice problems:** It is very unlikely that you will be successful in this course if you do not do the practice problems. Make the most of the time you spend on each practice problem by asking yourself: What are the concepts or skills being learned? What other similar questions could be asked on the topic? How would the solution/answer change if piece of information “X” in the statement of the problem was changed to “Y”? Could the problem be posed in more general/specific terms?

CALENDAR OF LECTURES

Please note that this calendar may change as the semester proceeds. The chapter numbers refer to the 11th edition of the textbook.

Date	Topics	Reading
Sep. 6	Introduction, Review of classical physics	Review C&J
Sep. 8	Review of classical physics (cont'd)	
Sep. 13	Review of classical physics (cont'd)	7A
Sep. 15	The origins of quantum mechanics	
Sep. 20	Wavefunctions	7B
Sep. 22	Operators and observables	7C
Sep. 27	Operators and observables (cont'd)	7D & 7E
Sep. 29	The quantum theory of motion	
Oct. 4	The quantum theory of motion (cont'd)	7F
Oct. 6	The quantum theory of motion (cont'd)	
Oct. 11	Exercises in class	
Oct. 13	Midterm Exam #1 (covers Chapter 7)	
Oct. 18	Hydrogenic atoms	8A
Oct. 20	Hydrogenic atoms (cont'd)	
Oct. 25	Many-electron atoms	8B
Oct. 27	Atomic spectra	8C
Nov. 1	Valence-bond theory, Molecular orbital theory	9A & 9B
Nov. 3	Molecular orbital theory: diatomic molecules	
Nov. 8	Molecular orbital theory: diatomic molecules (cont'd)	9D
Nov. 10	Molecular orbital theory: polyatomic molecules	9E
Nov. 15	Midterm Exam #2 (covers Chapters 8 and 9)	
Nov. 17	Molecular symmetry	10A
Nov. 22	General features of molecular spectroscopy	11A
Nov. 24	NO LECTURE	
Nov. 29	Rotational and vibrational spectroscopy	11B & 11C
Dec. 1	Rotational and vibrational spectroscopy (cont'd)	
Dec. 6	Electronic spectra, Decay of excited states	11F & 11G
Dec. 8	Electronic spectra, Decay of excited states (cont'd)	
Dec. 13	Exercises in class	
TBA	Final Exam (cumulative)	