

Chemistry 1410, Physical Chemistry 1, Fall 2023

Instructor: K. Jordan, 330 Eberly Hall; jordan@pitt.edu

Text: *Quantum Chemistry and Spectroscopy*, 4th edition, by Thomas Engel

Lectures: Tue. and Th., 1:00 PM – 2:15 PM, Room 150 CSC

Recitation: Wed., 2:00PM – 2:50 PM, Room 150 CSC

Office Hours: Tuesday 11:00 AM – 12:00 PM; Wed. 12:30 – 1:30 PM, 330 EH

Class web page: www.pitt.edu/~jordan/chem1410-f23

TA: The TA for the course, Gessica Adornato. Gessica's office hours are Tuesday 3:00 – 4:00 PM, Room 226 EH. She can be reached at email at GMA57@pitt.edu

Goals: In this course you will learn how about the key aspects of quantum mechanics, particularly those that are important in chemistry.

Grading: Two exams, two (30% each), homework (10%), presentation on research paper (25%), participation (5%)

Homework: Homework will be assigned on an approximately weekly basis and will be due one week after being assigned. Homeworks will provide you experience in applying concepts and methods that you learn to solving chemically relevant problems. In grading homeworks emphasis will be placed on approach and effort,

Exams: All exams are open book, i.e., you can use your text and notes, but no other sources. Makeup exams are permitted only in the case of medical emergencies.

Lectures: You are encouraged to read through lecture notes and the relevant material in the text in advance of lecture. The goal is to devote part of each lecture to discussion, and it would be useful if you come to each lecture with one or more questions that could serve as the basis for discussion.

Academic Integrity: Students in this course will be expected to comply with the University of Pittsburgh's Policy on Academic Integrity (<http://www.cfo.pitt.edu/policies/policy/02/02-03-02.html>). Any student suspected of violating this obligation for any reason during the semester will be required to participate in the procedural process, initiated at the instructor level, as outlined in the University Guidelines on Academic Integrity.

Use of Canvas: I expect to set up Canvas so that it can be used to submit Homeworks.

Use of Piazza: We will make use of the web-based Piazza gathering site. This allows students to post questions and for the instructors and other students to provide comments. In posting material, your identity will not be known to other students. The link is <https://piazza.com/pitt/fall2023/chem1410sec1300>.

Computational/numerical calculations: One of the easiest to use software packages for solving problems in Physical Chemistry is Wolfram Alpha. This is a web-based program. Anyone can use the basic Wolfram Alpha program, but to solve more complicated problems, you'll want to upgrade to the Pro version for which the University has a license. I will provide information on how to get the license for the Pro version.

Schedule:

Aug 29	Chapter 1, the need for quantum mechanics;
Aug 31, Sept 5	Chapter 2, the Schrödinger Equation
Sept 7, 12	Chapter 3, postulates of QM

Sept 14, 19	Chapter 4, QM of simple systems; Chapter 5, particle in the box
Sept 21, 26	Chapter 6, commuting operators
Sept 28, Oct 3	Chapter 7, QM of vibration and rotation; Exam 1 (Tues)
Oct 5, 10	Chapter 7, QM of vibration and rotation; Chapter 8, vibrational and rotational spectroscopy
Oct 12, 17	Chapter 9, the H atom
Oct 19	Chapter 10, many el. atoms; Chapter 11, atomic spectroscopy
Oct 24, 26	Chapter 12, H ₂ ⁺ and H ₂
Oct 31, Nov 2	Chapter 12, bonding in diatomics; Exam 2 (Thurs)
Nov 7, 9	Chapter 13, bonding in polyatomics (also some symmetry from Chpt. 16)
Nov 14, 16	Chapter 14, electronic spectroscopy
Nov 28, 30	Chapter 15, computational chemistry
Dec 5, 7	Preparation for Research Presentations
Dec 12	Research presentations (Tues)