

## Chemistry 56. Physical Chemistry II

**INSTRUCTOR:** Prof. Keith T. Kuwata, Olin-Rice 318, 696-6768, kuwata@macalester.edu.

Web page: [www.macalester.edu/~kuwata](http://www.macalester.edu/~kuwata) (for class handouts, class overheads, and answer keys)

**REQUIRED TEXT:** Peter Atkins and Julio de Paula, *Physical Chemistry*, 7th ed., W. H. Freeman, New York, 2002. (Lab instructions will be given in handouts.)

**OTHER REQUIRED MATERIALS:** Macalester College and the State of Minnesota both require that you wear safety goggles during all laboratory sessions. **You will not be allowed to work in lab if you do not bring your own pair of goggles.**

**DESCRIPTION:** This course offers a rigorous, mathematical, and microscopic treatment of atoms, molecules, and states of matter. In Unit 1, we begin with an empirical treatment of solid-state structure using the method of X-ray diffraction (Chapter 23). We then lay a foundation of perhaps the greatest scientific breakthrough of the 20th century--quantum mechanics (Chapters 11 and 12). In Unit 2, we apply the techniques of quantum mechanics to understand the electronic structure of atoms and molecules (Chapters 13 and 14). We also introduce elegant and powerful methods of group theory to describe the symmetry of molecules (Chapter 15). In Unit 3, we exploit both quantum mechanics and symmetry to discuss the interactions of electromagnetic radiation with molecules—that is, spectroscopy (Chapters 16, 17, and 18). Finally, we introduce the concepts of statistical mechanics, an actively-researched area that seeks to predict thermodynamic properties from the quantum-mechanical structure of matter.

**LECTURES:** MWF from 8:30 to 9:30 a.m. in Olin-Rice 301. It is your responsibility to do the assigned reading before lectures on the material begin. See pp. 3-4 of this syllabus for the approximate lecture schedule. Doing the reading will help you understand the lectures a lot more and prepare you to ask questions during class.

**LABORATORIES:** Thursdays from 8:30 to 11:40 a.m. in various rooms (see schedule). Like Chemistry 37 (Organic I), several of our lab sessions will be devoted to additional lecturing and the interpretation of spectra. Due to limited resources (*e.g.* we have only one FTIR spectrometer), you will need to do some work outside the “official” lab time. I will give you card access to the appropriate instrumental laboratories. **However, note that you must never work alone in any lab.** You will work in pairs of your choosing throughout the semester; be paired up by the first day of lab (January 30). I will generally provide handouts for a given lab session by Monday of that week.

**PROBLEM SETS:** Assignments (usually problems from your text) will usually be handed out a week before they are due (see pp. 3-4 for due dates). **There will be a 20% per day penalty for late homework, and will not be accepted after the test on that material.** Unless otherwise noted, each of the ten problems sets will be weighted equally in determining this percentage of your cumulative score. My solutions for the problems sets will be posted on the course web page to help you study.

Doing the assigned homework is essential for you to learn the material and do well on exams. However, do not expect the specific problems I assign to be a targeted rehearsal for, or preview of, test questions. The goal is for you to master concepts and principles on which you will be tested. Please come talk with me if you have any questions on the homework. You are encouraged to work with other

people, but what you turn in must be your own work. I also highly recommend you make time to do additional problems as you study for this course.

**EXAMINATIONS:** There will be three midterm tests consisting largely of quantitative and qualitative problems, along with a few multiple-choice questions. Each test will run two hours. All tests will be administered during the laboratory time slot in Olin-Rice 350. This will provide you the time to answer in-depth problems.

Your final will largely consist of an American Chemical Society standardized exam consisting of multiple-choice questions. This must be taken at the official time: Tuesday, May 8, 8:30–10:30 a.m. in OR 301.

**GETTING HELP:** I will be available in my office M 1:30-2:30 p.m., T 1:30-2:30 p.m., W 2:30-3:30 p.m., and Th 5:00-6:00 p.m. If you can't make one of these office hours, please make an appointment with me, or just come by—I'll usually be somewhere in Olin-Rice. Other helpful people include the class teaching assistant, Will Ames ([wames@macalester.edu](mailto:wames@macalester.edu), 698-4138) and tutors at the MAX Center. We are all eager to help you master the material in this course!

**GRADING: Homework: 20%      3 Tests: 40%      Lab Work: 20%      Final: 20%**

Grades will be assigned using a curve based on your cumulative percentage of points. However, everyone who earns at least 90% is guaranteed an A or an A-. Typically, if your cumulative score is close to the class average, you will receive a B—but this is not guaranteed. Note that I will not be assigning official (albeit non-permanent) midterm grades. However, I will be happy to estimate your grade for you at any time.

**ACADEMIC INTEGRITY:** Copying another pair's lab data, copying another person's lab report or homework (from this or past years), obtaining copies of tests prior to their administration, using unauthorized materials during tests, sharing or stealing information during an exam, and alteration of a graded exam and then requesting a re-grade all constitute cheating and are forbidden. As per the Macalester Student Handbook, I will report any clear violation of academic integrity standards to Ellen Guyer, the Dean of Academic Programs.

**COURSE SCHEDULE (timing of lecture topics may vary)**

<b>Date</b>	<b>Day</b>	<b>What's Due?</b>	<b>Chap</b>	<b>Topics/Event</b>
1/27	M		23	Solid State Structures; X-Ray Diffraction
1/29	W		23	
1/30	Th		Lab	Crystal Structures Worksheet (in OR 378)
1/31	F		23	
2/3	M	<b>PS 1</b>	23	XRD Lab Preview (with Petrology class, Karl Wirth)
2/5	W		11	Quantum Mechanics: Fundamental Concepts
2/6	Th		Lab	XRD Measurements (at a convenient time)
2/7	F		11	<b>[Validation Deadline]</b>
2/10	M		11	
2/12	W			XRD Lab Presentations (with Petrology class, Karl Wirth)
2/13	Th		Lab	To be announced
2/14	F	<b>XRD Report</b>	12	Quantum Mechanics: Applications <b>[Add/Drop Deadline]</b>
2/17	M	<b>PS 2</b>	Lab	The $\beta$ -Carotene Spectrum
2/19	W		12	
2/20	Th		12	Lecture (in OR 350)
2/21	F		12	
2/24	M	<b>PS 3</b>	13	The Electronic Structure and Spectra of Atoms
2/26	W		13	
<b>2/27</b>	<b>Th</b>			<b>TEST 1: Lectures thru 2/21; PS 1, 2, and 3 (in OR 350)</b>
2/28	F	<b><math>\beta</math>-Carotene</b>	13	
3/3	M		14	The Electronic Spectra of Molecules
3/5	W	<b>PS 4</b>	14	
3/6	Th		Lab	Assigning the Na Spectrum (in OR 350)
3/7	F		14	
3/10	M	<b>Na Spectrum</b>	14	
3/12	W		14	
3/13	Th		Lab	Assigning the K Spectrum (in OR 350)
3/14	F	<b>PS 5</b>	15	Molecular Symmetry and Group Theory
<b>3/15 – 3/23</b>			<b>Spring Break (no class)</b>	
3/24	M		15	
3/26	W	<b>K Spectrum</b>	15	
3/27	Th		Lab	The Huckel Model (in OR 350)
3/28	F		15	
3/31	M	<b>PS 6</b>	16	Rotational and Vibrational Spectroscopy
4/2	W		16	
<b>4/3</b>	<b>Th</b>			<b>TEST 2: Lectures thru 3/28; PS 4, 5, and 6 (in OR 350)</b>
4/4	F		16	<b>[Withdraw Deadline]</b>

<b>Date</b>	<b>Day</b>	<b>What's Due?</b>	<b>Chap</b>	<b>Topics/Event</b>
4/7	M	<b>Huckel</b>	16	
4/9	W		16	
4/10	Th		Lab	Computational Chemistry (in OR 341)
4/11	F	<b>PS 7</b>	17	Electronic Spectroscopy
4/14	M		17	
4/16	W		17	
4/17	Th	<b>Computation</b>	Lab	The FTIR Spectrum of HCl (in OR 378)
4/18	F			<b>Good Friday (no class)</b>
4/21	M	<b>PS 8</b>	18	Magnetic Resonance Spectroscopy
4/23	W		18	
4/24	Th		Lab	To be announced
4/25	F	<b>FTIR</b>	18	
4/28	M	<b>PS 9</b>	19	Statistical Thermodynamics: Fundamentals
4/30	W		19	
<b>5/1</b>	<b>Th</b>			<b>TEST 3: Lectures thru 4/25; PS 7, 8, and 9</b>
5/2	F		19	
5/5	M	<b>PS 10</b>	20	Statistical Thermodynamics: Applications
<b>5/8</b>	<b>Th</b>			<b>FINAL EXAMINATION, 8:30 - 10:30 a.m., OR 301</b>
5/9	F	<b>Final Lab</b>		