Lewis & Clark College
Physical Chemistry: Quantum Chemistry/Statistical Mechanics
Chemistry 320
Fall, 2006

Basic Information

Professor: Barb Balko; Olin 225; x 7534; balko@lclark.edu

Department Secretary: Linda Noble; Olin 226A; x 7530; noble@lclark.edu

Tentative Office Hours: T and Th: 9 – 11 am; also, by appointment

Lectures: MWF, 11:30 – 12:30, Olin 102

Class Website: www.lclark.edu/~balko/chem320.htm; some material may be on WebDisk (http://webdisk.lclark.edu)

Class Listserver: 06FA-CHEM-320-01@lclark.edu

Required Texts: Engel, *Quantum Chemistry & Spectroscopy*
Chang, *Physical Chemistry for the Chemical and Biological Sciences*

"Reserve" Texts: I have many texts on quantum chemistry and the mathematics used in quantum chemistry. These texts could be used for additional practice problems or to see a different discussion of material. Please come see me if you'd like to look through or borrow one of these books.

General Information

We will spend the bulk of this semester covering quantum chemistry—applying quantum mechanics to chemical problems. Quantum mechanics was developed during the early twentieth century as scientists began to realize that classical mechanics could not correctly describe the behavior of very small particles such as electrons. During the semester, we will learn how to carry out quantum mechanical calculations and approximations. We will apply what we learn to spectroscopy—a way to visualize the quantum nature of molecules. During the last week or so of the semester, we will introduce statistical mechanics. This is a nice transition to thermochemistry (the focus of Chem310) since statistical mechanics shows us how to sum all the quantum mechanical behavior of atoms and molecules to allow us to predict bulk behavior (i.e., thermodynamics). Statistical mechanics provides the connection between quantum mechanics and thermodynamics.

Lectures:
It is important to read your textbook before coming to class. Use the syllabus to find out what will be covered in lecture and read ahead. When you go home after class, do some problems to see if you can apply what you learned that day. I will often assign problems that we will go over during the next lecture to force you to do this. If you don't

understand something, ask questions during lecture or come see me after class or during my office hours.

Office Hours:

If you have questions that cannot be answered in class, would like additional practice problems, would like to review some mathematics, or would like to talk about chemistry in general, please see me during my office hours. If these times don't work for you, feel free to make an appointment with me for another time. I plan to use my Tuesday office hours as a problem-solving session; you can work on problems during this time (either homework problems or additional problems that I provide) in a group setting with me available for assistance.

Class Website:
The class website will feature pdf files of homework assignments and solutions to homework problems. There will also be links to other sites that you may find interesting. If the site starts to get full, older files will be moved to WebDisk.

Academic Honesty:
I expect academic honesty. This means homework and exams should be your own efforts. Discussion about homework assignments is encouraged but the work you turn in should be your own (i.e., it should be in your own words and you should be able to explain it fully if asked). Cheating will result in failure on the assignment, possible failure of the course, and disciplinary action by the College Honor Board. Please consult the *Pathfinder* for more information on the College's academic integrity policy. If you are having problems come see me!

Academic Accomodations:
If you have a disability that may impact your academic performance, you may request accommodations by submitting documentation to the Student Support Services Office in Albany Quadrangle (x7191). That office will notify me of the accommodations for which you are eligible.

Grading

3 "Midterm" Exams	50%
Homework	20%
Final Project	10%
Final	20%

Midterm Exams
Three one hour midterms will be given in class. The *approximate* dates are given in the syllabus.

Homework
Homework will be assigned approximately once a week; some of the assignments will involve computer calculations and class presentations. I will drop your lowest score when I calculate your homework grade. Homework will be accepted up to 1 week late (with a 10% penalty).

Final Project
Throughout the semester we will have the opportunity to use computer calculations to help visualize electron density and molecular geometries. For the final project, I would like each student to expand on one of these calculations and present the results to the class during the last week of class. Your grade will be based on written work as well as the presentation.

Final Exam
Your final exam is scheduled for Monday, Dec. 18, 1:00 – 4:00 PM.

Tentative Class Schedule

Date	Material Covered	Reading
Wed., Sept. 6	introduction, blackbody radiation, photoelectric effect	Engel: 1.1 – 1.4; Chang: 14.2 – 14.3
Fri., Sept. 8	de Broglie's postulate, diffraction, atomic spectra	Engel: 1.5 – 1.7; Chang: 14.4 – 14.5
Mon., Sept. 11	wave-particle duality; classical picture of waves	Engel 2.1 – 2.4; Chang: 14.1
Wed., Sept. 13	Schrödinger equation, operators, observables, eigenfunctions, eigenvalues	Engel: 2.5 – 2.7; Chang: 14.7
Fri., Sept. 15	quantum mechanical postulates	Engel: 3.1 – 3.5; Chang: 14.7
Mon., Sept. 18	particle-in-a-box	Engel: 4.1 – 4.2; Chang: 14.8
Wed., Sept. 20	particle-in-an-n-dimensional box	Engel: 4.3 – 4.4
Fri., Sept. 22	applications of particle-in-a-box	Engel: 5.1 – 5.8; Chang: 14.9
Mon., Sept. 25	uncertainty principle	Engel: 6.1 – 6.5; Chang: 14.6
Wed., Sept. 27	harmonic oscillator (classical and quantum mechanical)	Engel: 7.6, 7.1
Fri., Sept. 29	rigid rotator	Engel: 7.7, 7.2 – 7.3
Mon., Oct. 2	**Exam 1 (Engel Chapters 1 - 6)**	
Wed., Oct. 4	angular momentum	Engel: 7.4 - 7.5, 7.7 – 7.8
Fri., Oct. 6	spectroscopy basics	Engel: 8.1 – 8.2; Chang: 17.1
Mon., Oct 9	selection rules and vibrational spectroscopy	Engel: 8.3 – 8.5
Wed., Oct. 11	rotational spectroscopy and vibrational-rotational spectroscopy	Engel: 8.6 – 8.8
Fri., Oct. 13	**Fall Break**	

Mon., Oct. 16	the hydrogen atom	Engel: 9.1 – 9.3; Chang: 14.10
Wed., Oct. 18	the hydrogen atom, continued	Engel: 9.4 – 9.6
Fri., Oct. 20	many-electron atoms	Engel: 10.1; Chang: 14.11
Mon., Oct. 23	the Pauli principle	Engel: 10.2 – 10.3
Wed., Oct. 25	approximation methods	Engel: 10.4 – 10.6
Fri., Oct. 27	orbital and spin angular momentum	Engel: 10.7 – 10.10
Mon., Oct. 30	atomic spectroscopy, lasers	Engel: 11.1, 11.3 – 4, 11.6; Chang: 17.4, 17.8
Wed., Nov. 1	quantum mechanics description of H_2^+	Engel: 12.1 – 12.5
Fri., Nov. 3	**Exam 2 (Engel Chapters 8 – 10)**	
Mon., Nov. 6	quantum mechanics description of H_2	Engel: 12.6 – 12.7; Chang 15.1 – 15.2
Wed., Nov. 8	molecular orbitals for diatomics	Engel: 13.1 – 13.8; Chang: 15.5 - 15.6
Fri., Nov. 10	hybridization	Engel: 14.1 – 14.2, 14.4 – 14.5; Chang: 15.3, 15.5
Mon., Nov. 13	molecular spectroscopy	Engel: 15.1 – 15.4
Wed., Nov. 15	excitation with UV-Vis, fluorescence, and phosphorescence	Engel: 15.5 – 15.8; Chang: 17.7
Fri., Nov. 17	computational chemistry	Engel: 16.1 – 16.7
Mon., Nov. 20	computational chemistry, continued	Engel: 16.8 – 16.10
Wed., Nov. 22	NMR Spectroscopy	Engel: 18.1 – 18.10, 18.14; Chang: 17.5

Fri., Nov. 24	**Thanksgiving Break**	
Mon., Nov. 27	statistical mechanics: microstates and entropy	Chang: 23.1
Wed., Nov. 29	statistical mechanics: Boltzmann distribution	Chang: 23.2
Fri., Dec. 1	**Exam 3 (Engel Chapters 11 – 16, 18)**	
Mon., Dec. 4	presentations; statistical mechanics: partition functions	Chang: 3.8, 23.3 – 23.4
Wed., Dec. 6	presentations; statistical mechanics: thermodynamic quantities	Chang: 23.5
Fri., Dec. 8	presentations; statistical mechanics: equilibrium and transition state theory	Chang: 23.6 - 23.7
Mon., Dec. 11	review	
Mon., Dec. 18	**Final (1 – 4 pm)**	