Chemistry 310 - Physical Chemistry II
Spring 2007

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Office Hours: I am generally at school from 9:00 A.M. to 6:00 P.M. every day, and often later. You may come by my office any time you wish. If I cannot work with you immediately, I will make an appointment to meet with you later, if possible later that day.

Prerequisites: Math 212 and Physics 132. Math 235 (Calculus III) and Math 240 (Differential Equations), while not required, are strongly recommended.

Texts:

Required: Peter Atkins and Julio DePaula, Physical Chemistry, Eighth Edition, W. H. Freeman, New York, 2002

Ira N. Levine, Quantum Chemistry, Fifth Edition, Prentice Hall, Inc., New York, 2000

John R. Taylor, An Introduction to Error Analysis, Second Edition, University Science Books, 1997

Recommended: Physical Chemistry requires a lot of mathematics. You should have a solid command of introductory calculus. Many of you will need to refer to your calculus book for help with differentiation and integration. In addition, we will be using mathematics beyond Math 211-212. In each case I will teach you the necessary math, but many of you will find it useful to have a reference available. The bookstore carries two inexpensive series which you may find helpful. They are the Schaum Outline Series, which includes volumes on Calculus, Differential Equations, Partial Differential Equations, Linear Algebra, and Advanced (Multivariable) Calculus, and the Essentials Series, which includes three volumes on Calculus, two on Differential Equations, and one on Linear Algebra. At the very least you should have either your book from Mathematics 211-212 or the Schaum Outline volume on Calculus.

Tentative Course Schedule: This semester we will be devoting most of our time to quantum chemistry, the detailed microscopic treatment of the structure of atoms and molecules and the methods for determining these structures. Much of our emphasis on quantum chemistry will be on applications to molecular spectroscopy. We will also be studying the basics of chemical kinetics. If time

allows, we will also study some statistical mechanics, and transition state theory.

Our tentative course schedule is: (QC = Quantum Chemistry, PC = Physical Chemistry)
(You can now tell your parents that your chemistry professor insisted that everything about his course be PC.)

Date	Topic	Sections
1/15	Introduction to Syllabus; Blackbody Radiation	PC: 8.1 QC: 1.1-1.2
1/17	Photoelectric Effect, Rydberg Spectra, Angular Momentum	PC: 8.1 QC: 1.2
1/19	Bohr Model, Photon Momentum, Wave-Particle Duality, Uncertainty Principle	PC: 8.1-8.2, 8.6 QC: 1.2-1.3
1/22	Dr. Abrash Out of Town: No Class	
1/24	Introduction to the Schrodinger Equation; Complex Numbers; Born Interpretation, Normalization	PC: 8.3, 8.4 QC:1.5, 1.6, 1.7
1/26-1/29	First Postulate, Operators; Second Postulate; Link Between Operators and Observables, Commutation	PC: 8.5, 8.7 QC: 3.1, 3.2, 3.3
1/31	Free Particle, Particle in a 1-D Box, Boundary Values, Application to Spectra of Conjugated Molecules	PC: 9.1 QC: 2.2, 2.3
2/2	Properties of Eigenfunctions, Degeneracy, Discrete and Continuous Probability Distributions, Fourth Postulate, Quantum Mechanical Averages	PC: 8.5, 8.7 QC: 3.2, 3.6, 3.7
2/5	Particle in a Three Dimensional Box, Multiple Integrals, Separation of Variables, Symmetry and Degeneracy	PC: 9.2, 9.3 QC: 3.5
2/7	Classical Harmonic Oscillator. Quantum Mechanical Harmonic Oscillator	PC: 9.4, 9.5 QC: 4.2, 4.3
2/9	Test One	
2/12	Rigid Rotor, Hamiltonian in Spherical Coordinates, Rigid Rotor Wavefunctions - Spherical Harmonics, Rigid Rotor Eigenvalues	PC: 9.7 QC: 6.1-6.4
2/14	Angular Momentum in Three Dimensions. Quantum Mechanical Treatment of Angular Momentum, Rigid Rotor and Bond Length	PC: 9.7 QC: 5.2-5.3
2/16	Time Dependent Schrodinger Equation. Review of Postulates	PC: 8.3 QC: 1.5
2/19-2/21	Hydrogen-Like Atom, Eigenfunctions, Energy Eigenvalues, Appearance of Orbitals, Angular Momentum	PC: 10.1-10.2 QC: 6.5-6.8
2/23	Perturbation Theory, Zeeman Effect	PC: 9.9 QC: 9.1
2/26	He Hamiltonian, Three Body Problem, Variational Method	PC: 10.7 QC: 8.1-8.2
2/28	He Atom Eigenvalues, Effective Nuclear Charge	QC: 8.1, 8.2,

3/2	Electron Spin, Spin Wave Functions, Effect of Spin on Energy	PC: 9.8, 10.4 QC: 10.1, 10.2
3/3-3/11	Spring Break	
3/12	Pauli Exclusion Principle, Symmetry of Wavefunctions, Indistinguishability of Electrons, Postulate 6, He Excited States	PC: 10.4 QC: 10.3-10.5
3/14	Slater Determinants	QC: 10.6
3/16	Test Two	
3/19	The Hartree-Fock Approximation	PC: 10.5 QC: 11.1, 11.3
3/21-3/23	Term Symbols; Hund's Rule; Periodic Properties	PC: 10.9 QC: 11.5
3/26	Periodic Properties	PC: 10.6 QC: 11.2
3/28	H_2^+ Hamiltonian, Born-Oppenheimer Approximation, Bound and Repulsive Potentials. Comparison Between H_2 and H_2^+ Bound Potentials	PC: 11.1 QC: 13.1-13.3
3/30	LCAO Approach to H_2^+	PC: 11.3, 11.4 QC: 13.4-13.6
4/2	LCAO Approach to H_2; Other H_2^+ Molecular Orbitals, Naming Molecular Orbitals, Molecular Orbital Energy Diagram	PC: 11.4 QC: 13.6, 13.7, 13.9
4/4	Molecular Term Symbols, Basic MO Treatment of Homonuclear Diatomics and Heteronuclear Diatomics	PC: 11.4, 11.5 QC: 13.8
4/6	Valence Bond Theory, Hybridization	PC: 11.1, 11.2 QC: 13.10, 13.11
4/9	Huckel M.O. Theory	PC: 11.6 QC: 16.3
4/11-4/13	Electronegativity, Ionic Bonding, Dipole Moments, Intermolecular Forces, Lennard Jones Potential, Hydrogen Bonding	PC 11.8
4/16	Test Three	
4/18	Spectroscopy and Electromagnetic Radiation, Rotational Spectra	PC: 13.4-13.6. 13.8
4/20-4/25	Vibrational Spectra, Thermal Population of Vibrational and Rotational Levels, Vibrational-Rotational Spectroscopy Centrifugal Distortion, Anharmonicity; Vibrations of Polyatomic Molecules, Vibrational Selection Rules,	PC: 13.9-13.15
4/27	Electronic Spectroscopy	PC: 14.1-14.2

Tentative Test Schedule

There will be three hour exams and a final exam. The three one hour exams are scheduled for February 9th, March 16th, and April 16. Tests will cover all material up to the day of the exam.

The final exam is scheduled on Wednesday, May 2nd, from 2:00 P.M. to 5:00 P.M.. In addition, students may self schedule the exam on either Monday, April 30th, or Tuesday, May 1st.

Grading

Homework, the one hour exams, a final exam and the laboratory will be the basis for the course grade. The weighting for each of these components is as follows:

Homework:	10%
Three One Hour Tests:	45%
Final Exam:	20%
Laboratory	25%
Extra Credit: Notebook	Up to 3.5 points added to your final grade.

The grades for each of the one hour exams and the final exam will be based on a modified curve. This means that a traditional bell curve grading distribution will be my lower limit. If, for example, on examining the papers which would correspond to a C on the tradition curve, I feel that they are B work I will modify the curve to reflect this. I have no objection to assigning all A's if everyone does excellent work. Since both the laboratory and lecture parts of the course are important, you must pass both sections of the course individually in order to pass the overall course. Thus someone with an A+ in the lecture part of the course who gets an F in the laboratory will get an F in the course.

Please note that all assignments are due in my office by 5:00 PM on the final day of classes.

Homework

Regular completion of homework problems is essential in mastering physical chemistry. This is especially true since it will take time and practice for you to translate mathematical expressions into physical and chemical intuition.

Homework this semester will be a selection of problems from Atkins and Levine. You are to attempt to complete all problems. After you have completed a problem or worked until no further progress is possible, having worked at least 20 minutes on the problem, compare your results with at least one other person in the class, and try to work it out together. If this fails, look up the answer in the solution manual on reserve in the library. Then mark on your homework report the problem number, the time spent, the person you consulted with and whether the problem was worked correctly.

Homework will be due each Monday at the beginning of class. Every one who attempts all problems for the week and turns in their homework report on time will receive full credit. Late reports will not be accepted. It is particularly important that you be completely frank about whether or not you have successfully completed a problem: it won't hurt your grade and it may be my only clue that you need help.

Collaboration on the problems from Atkins, and from Levine. A group of three to four people working together and discussing both the lecture materials and the problems together is often ideal. Talking through material is an excellent way to improve your comprehension or to zero in on areas in need of clarification. However, each of you knows how she or he works best and you should work in the way that you are most comfortable.

Attendance

You are expected to attend class. You are responsible for all material covered in class. If you miss a lab for what I deem a valid reason (illness, etc), I will try to arrange for you to make up the lab. No test makeups will be given. A missed test will count zero unless you are excused for a valid reason. I will determine the validity of the excuse. If you miss a test but are excused, the next test will count double. Please let me know if you have advance knowledge of missing a test or a lab.

Honor Code

The Richmond College and Westhampton College Honor Codes are very special and have the full support of this department. You will be expected to sign an honor pledge on each test. We expect that behavior in this class will be consistent with this code. To aid in this I would like to clarify certain issues. Collaboration on homework is allowed and encouraged. Group discussions of laboratories are allowed and encouraged, but no collaboration is allowed on the writing of the reports. Each report must be your creative, original contribution on the subject. To clarify, you may work together on calculations, and in the course of developing an understanding of the subject matter of the labs. Extensive discussion will be permitted. However, writing the lab report should be an individual effort.

To avoid plagiarism, any material in a lab report that is quoted directly from another source, such as a professional journal, must be cited. In addition, the sources of any data not measured by you and even ideas not originating with you must be cited. Exceptions would be equations like $F=ma$ or $E=mc^2$ which by now are common knowledge. Guidance on citations may be gained by looking at recent articles of the Journal of Physical Chemistry or the Journal of Chemical Physics in the Library. If you have any doubt about whether a citation is necessary, please feel free to consult with me.