Chemistry 310 - Physical Chemistry II
Spring 2019

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Office Hours: I am generally at school from 9:30 A.M. to 5:30 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 (or equivalent). Math 235 (Calculus III) and Math 240 (Differential Equations), while not required, are strongly recommended.

Texts:

Required: (if you are continuing from Chem 309, Fall 2018, the book we used in the Fall) Peter Atkins and Julio DePaula, Atkins' Physical Chemistry, 11th Edition, Oxford University Press, Oxford, UK, 2018. ISBN 10 = 0-19-876986-6

(if you did not take Chem 309, Fall 2018) Peter Atkins and Julio DePaula, Physical Chemistry: Quantum Chemistry, Spectroscopy and Statistical Thermodynamics, (This is volume 2 of the book. Check the ISBN before you buy to make sure you have the correct volume) 11th Edition, Oxford University Press, Oxford, UK, 2018. ISBN-10 = 0-19-881790-8

(for all Chem 310 students) Donald A. McQuarrie, Quantum Chemistry, Second Edition, , University Science Books, Mill Valley, California, 2008. ISBN 10 = 1-891389-50-4. Note that this is available both as a hardcover book from the bookstore or other booksellers, or as an e-book for purchase or rental from RedShelf.com at a much lower cost.

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. There is an inexpensive series which you may find helpful. It is the Schaum Outline Series, which includes volumes on Calculus, Differential Equations, Partial Differential Equations, Linear Algebra, and Advanced (Multivariate) Calculus. 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. We will conclude with applications to molecular spectroscopy.

Our tentative course schedule is:

Date	Topic	Sections
1/14	Introduction to Syllabus; Blackbody Radiation	Atkins 7A.1(a); McQuarrie1.1-1.2
1/16	Photoelectric Effect, Rydberg Spectra, Review of Angular Momentum	Atkins 7A.1(c); McQuarrie 1.3, 1.5-1.7
1/18	Bohr Model, Photon Momentum, Wave-Particle Duality, Uncertainty Principle	Atkins 7A.2(a), 7A.2(b), 7C.3; McQuarrie 1.8, 1.10-1.14
1/21	Martin Luther King Day Celebration – No Class (Dr. Abrash will be giving two ½ hour concerts of Civil Rights songs)	
1/23	Introduction to the Schrodinger Equation, Complex Numbers; Born Interpretation, Normalization	Atkins 7B; McQuarrie MathChapter A, 3.1, 3.4, 3.6
1/25-1/28	First Postulate, Operators; Second Postulate; Link Between Operators and Observables, Third Postulate, Commutation	Atkins 7C.1, 7C.4; McQuarrie 3.2, 3.3, 4.1-4.5
1/30	Free Particle, Particle in a 1-D Box, Boundary Values, Application to Spectra of Conjugated Molecules	Atkins 7D.1, 7D.2, McQuarrie 3.5
2/1	Properties of Eigenfunctions, Degeneracy, Discrete and Continuous Probability Distributions, Fourth Postulate, Quantum Mechanical Averages	Atkins 7C.2, McQuarrie 3.7,3.8, 4.6-4.8
2/4	Particle in a Three Dimensional Box, Multiple Integrals, Separation of Variables, Symmetry and Degeneracy	Atkins 7D.3; McQuarrie 3.9
2/6	Classical Harmonic Oscillator. Quantum Mechanical Harmonic Oscillator	Atkins 7E, McQuarrie 5.1-5.8
2/8	Rigid Rotor, Hamiltonian in Spherical Coordinates, Rigid Rotor Wavefunctions - Spherical Harmonics, Rigid Rotor Eigenvalues	Atkins 7F.1, 7F.2(a), 8C.2(b); McQuarrie 6.1, 6.2, 6.6
2/11	Angular Momentum in Three Dimensions. Quantum Mechanical Treatment of Angular Momentum, Rigid Rotor and Bond Length	Atkins 7F.2(b); McQuarrie Ch. 6 Appendix, 6.8
2/13	Time Dependent Schrodinger Equation. Review of Postulates	McQuarrie 4.9
2/18	Test One	
2/15-2/20	Hydrogen-Like Atom, Eigenfunctions, Energy Eigenvalues, Appearance of Orbitals, Angular Momentum	Atkins 8A; McQuarrie 7.1-7.3
2/22	Perturbation Theory, Zeeman Effect	McQuarrie 8.4, 8.5, 7.4

2/25	He Hamiltonian, Three Body Problem, Variational Method	Atkins 8B.1(a), 9D.2; McQuarrie 7.9, 8.1-8.3
2/27	He Atom Eigenvalues, Effective Nuclear Charge	Atkins 8B.3(a), McQuarrie 9.1, 9.2
3/1	Electron Spin, Spin Wave Functions, Effect of Spin on Energy	Atkins 8B.2(a); McQuarrie 7.5
3/4	Pauli Exclusion Principle, Symmetry of Wavefunctions, Indistinguishability of Electrons, Postulate 6, He Excited States	Atkins 8B.2(b), McQuarrie 9.4
3/6	Slater Determinants	McQuarrie 9.5
3/8	The Hartree-Fock Approximation	Atkins 8B.4, McQuarrie 9.3, 9.6-9.8
3/9-3/17	Spring Break	
3/18-3/20	Term Symbols; Hund's Rule	Atkins 8B.3(b), 8C, McQuarrie 7.6, 9.9-9.13
3/22	Periodic Properties	Atkins 8B.3(c)
3/27	Test Two	
3/25	H_2^+ Hamiltonian, Born-Oppenheimer Approximation, Bound and Repulsive Potentials. Comparison Between H_2 and H_2^+ Bound Potentials	Atkins Focus 9 Prologue; McQuarrie 10.1-10.2
3/29	LCAO Approach to H_2^+	Atkins 9B; McQuarrie 10.3-10.4
4/1	LCAO Approach to H_2; Other H_2^+ Molecular Orbitals, Naming Molecular Orbitals, Molecular Orbital Energy Diagram	Atkins 9C.1(a)-(b); McQuarrie 10.7-10.8
4/3	Molecular Term Symbols, Basic MO Treatment of Homonuclear Diatomics and Heteronuclear Diatomics	Atkins 9C.1(c), 9C.2; McQuarrie 11.1-11.4
4/5	Valence Bond Theory, Hybridization	Atkins 9A; McQuarrie bottom of page 530
4/8	Hückel M.O. Theory	Atkins 9E.1, 9E.2; McQuarrie 11.6-11.8
4/10-4/12	Electronegativity, Ionic Bonding, Dipole Moments, Intermolecular Forces, Lennard Jones Potential, Hydrogen Bonding	Atkins 9D.1
4/15	Spectroscopy and Electromagnetic Radiation, Rotational Spectra	Atkins 11A, 11B
4/17-4/19	Vibrational Spectra, Thermal Population of Vibrational and Rotational Levels, Vibrational-Rotational Spectroscopy Centrifugal Distortion, Anharmonicity; Vibrations of Polyatomic Molecules, Vibrational Selection Rules,	Atkins 11C, 11D, 11E
4/22	Test Three	
4/24-4/26	Electronic Spectroscopy	Atkins 11F

<u>Tentative Test Schedule</u>

There will be three hour exams and a final exam. The three one hour exams are scheduled for February 18th, March 27th, and April 22rd Tests will cover all material up to the day of the test.

The final exam is scheduled on Tuesday, April 30th, from 9:00 A.M. to 12:00 Noon. There are also opportunities to self-schedule the final. Students may self-schedule their finals during any daytime exam period (i.e., 9:00 A.M. or 2:00 P.M.) between Monday, April 29th and the 2:00 P.M. slot on Friday, May 3rd.

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:	15%
Three One Hour Tests:	60%
Final Exam:	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. Please note that all assignments except the extra credit notebooks are due in my office by 5:00 PM on the final day of classes. Since the extra credit notebooks are useful as a study aid, you may keep them until you take your final exam.

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 DePaula and McQuarrie. 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. 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 Wednesday 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, unless the work was completed on time. If you tell me that it was completed on time, and that you just forgot to bring it or turn it in I will accept that statement as pledged and accept the work without penalty. 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 is recommended. 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. I cannot emphasize enough the importance of group work. People who do group work regularly always succeed at a higher level than those who don’t.

However, each of you knows how she or he works best and you should work in the way that you are most comfortable.

Extra Credit Notebook

I am offering the option for everyone in the class to keep an extra credit notebook. The notebook will be on your assigned reading both in Atkins , DePaula, and Keeler and in McQuarrie. It is a learning-through-writing exercise called a double-entry notebook. To complete the notebook, you will divide each page of some kind of bound notebook into two columns. In the left hand column, you will write a brief summary paragraph of each assigned section of the reading. The paragraph should not consist of your notes on the reading. Rather, you should read the section, and then summarize the essential content of the section in your own words, in full sentences. If a chapter consists of nine sections, there should be nine separate summary paragraphs. A good summary will not be a list of topics (This section discussed blackbody radiation, the photoelectric effect and the ultraviolet catastrophe.) but rather should be a summary of the essential content (i.e. At the turn of the century a number of experiments were performed which could not be explained by either Newtonian mechanics or the electromagnetic theory of Maxwell. These included blackbody radiation, a phenomenon in which …") If you do a good job on the summary section (well written paragraphs and all sections covered in class done) you'll earn at least a B+ on the notebook. Please note that substantially incomplete notebooks will receive little or no credit.

The second column in the extra credit notebook will be the reflection section. In the reflection section, you'll be writing things that the section makes you think of. It could be "I don't get this." (Hopefully not too often.) It could be, "This reminds me of XXX I read in general chemistry, but is deeper and more subtly expounded." It could be along the lines of "If this is true, then perhaps it implies this" Reflections are not required for every section of the reading, but should be done for a majority of the sections. Doing an excellent job on reflections can raise your notebook grade into the A- to A+ range. An A+ will receive 3.5 points added on to your final average, an A 3 points, an A- 2.5 points, and so on.

Attendance

You are expected to attend class. You are responsible for all material covered in class. 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 rest of the material in the class will simply count proportionately more. 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 have my full support and 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. Please note that since collaboration on homework is strongly encouraged that you may collaborate on Chem 310 homework assignments as much as you wish without violating the honor code.