Physical Chemistry II

Instructor Prof. William R. Simpson

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Class meeting Monday, Wednesday, and Friday 10:30 - 11:30 AM, REIC 165

Laboratory Tuesday, 11:30 – 2:30 PM, REIC 245 (sometimes in Chemistry computer lab,

Section REIC 172)

Office hours Mon, Fri 11:30AM—12:30PM, Tu 10:30-11:30AM, and by appointment Text "Elements of Physical Chemistry" by Atkins and de Paula, 7th edition

Handouts for laboratory section

Credits 4 credits, 3 hours of lecture, 3 hours of laboratory

Requirements Textbook, internet access (can use REIC 172 computer laboratory)

<u>Course Description (from catalog)</u>: Atomic and molecular structure, and spectroscopy, and statistical mechanics. Course teaches these concepts using both lecture and laboratory instruction. Special fees apply. Prerequisites: CHEM F331; MATH F253X; or permission of instructor. (3+3)

<u>Course Goal</u>: Chemistry 332 is the second semester of a two-semester series in physical chemistry. Our goal is to understand how physical and mathematical theories can be used to explain chemical behavior.

<u>Learning Outcomes:</u> In this semester, you will study quantum mechanics with applications in atomic and molecular structure, spectroscopy, and statistical themodynamics. At the end of the course, successful students will be able to:

- Apply quantum mechanical concepts to translation, rotation, and vibration of molecules.
- Describe shapes of atomic and molecular orbitals and use them to explain chemical bonding.
- Relate atomic and molecular spectra to electronic structure and molecular shape.
- Use molecular energy levels to predict bulk properties through statistical thermodynamics.

Course type/structure: This is an in-person class with integrated laboratory and follows the schedule of topics on the last page of this syllabus. Specific reading assignments for each coming class will be posted to the Blackboard course management system within a few hours of the end of the prior class. In classes, I will lecture on the material, answer questions, and may have students interact through problem solving or discussions. Reading the book **before** the lectures will be important for following and understanding the lectures. The Monday classes are a combination of lecture and in-class quizzes. These Monday quizzes are a very important part of the course as they will help you to stay current with and to understand the material of the course. The course also has a laboratory section to give physical examples of the concepts you learn in class.

<u>Grading Structure (points)</u>: Your course grade will be based on the total points of the hour exams, the final exam, the quiz scores, reading questions, laboratory (see below), and possibly extra credit from reading questions (see below). Material assigned in readings, in lecture, in laboratory, or in homework problems may appear on an exam. The maximum number of points for each is given below:

Exercise	Points
Hour exams (100 points each)	300
Final exam	100
Quizzes	80
Reading questions	20
Laboratory	150
Total	650
Extra credit: Reading questions	+10

Exams: The exams will be given during class, and will be one hour in length. You are permitted to use a calculator, a unit sheet (distributed with the exams), and a half sheet of paper (8.5"x5.5") containing only formulas. You should continually prepare this formula sheet as you study the material. Don't copy your friend's sheet. Preparing and organizing material is essential. I will look at the sheet during the exam and may collect the sheet. Chemistry Department regulations require that any student caught cheating on graded work will be assigned a course grade of F. Course drop forms will not be signed in these cases. Homework, quiz, and exam solutions will be **posted on the web in the Blackboard system**.

<u>Make up exams</u>: Make-up exams will be allowed if you have a good reason. If you anticipate an absence (work commitments, intercollegiate sports), talk to me **before** the exam to make arrangements. If the absence is unexpected (illness, family or personal difficulties), talk with me at the earliest possible opportunity.

Nondiscrimination policy: Every qualified student is welcome in my classroom. As needed, I am happy to work with you, disability services, veterans' services, rural student services, etc. to find reasonable accommodations. Students at this university are protected against sexual harassment and discrimination (Title IX), and minors have additional protections. As required, if I notice or am informed of certain types of misconduct, then I am required to report it to the appropriate authorities. For more information on your rights as a student and the resources available to you to resolve problems, please go the following site: www.uaf.edu/handbook/

<u>Disability Services:</u> Students with documented disabilities who may need reasonable academic accommodations should discuss these with me during the first two weeks of class. You will need to provide documentation of your disability through the UAF Office of Disability Services. For more information, contact Disability Services at <u>uaf-disabilityservices@alaska.edu</u>, 474-5655 or by TTY at 474-1827 or http://www.uaf.edu/disability.

<u>Syllabus Revision:</u> Before the drop date, I may slightly revise the syllabus to correct errors that are found. Revision at a later time would require approval by all students in the class at that time. A revised copy of the syllabus will be distributed to all students and posted to Blackboard. Adjustments to the tentative lecture pacing and/or laboratory order below can be made by the instructor to best optimize use of class / lab time and will be communicated to students via Blackboard and email.

<u>Homework:</u> Physical chemistry is a hard class, which you will only learn by doing homework and thinking deeply about it. Every week you will be assigned 3 to 6 homework exercises. These homework exercises are not graded, but you will be provided with homework keys (posted on the web). If you attempt a problem but don't get an answer, see me for help. A few of these exercises are selected to improve your mechanical skills and also help you to find the right formula to apply to a problem. Many of the problems will be conceptual in nature. These questions address the theoretical connections between various physical chemistry problems.

Quizzes: The quizzes will be given during class on Mondays and will be about 15 minutes in length. You are permitted to use a calculator, and a formula / unit sheet (distributed with the

quiz). The formula / unit sheet will have all appropriate formulae as well as numerical values for constants and unit conversions. The quizzes will be on all Mondays except on the Monday following the week of an hour exam (see schedule). The purpose of the quiz is to provide a frequent check on learning progress. Doing the homework diligently is the best way to assure good grades on the quizzes, and past experience has shown that good quiz grades translate to good course grades. There will be no makeup quizzes, but your three-lowest quiz grades will be dropped. Answers to the quizzes will be posted on the website.

Working in groups: While working on your homework and/or preparation for Monday quizzes, you may work in groups. In fact, working in groups usually results in faster and deeper learning. Whether you work in a group or alone, you must take the exams and quizzes alone. Copying the solution of another student is not working in a group and will lead to a hole in your understanding that will appear in your exam and quiz performance. My advice is to work the homework and study in groups but don't cheat yourself.

Reading Assignments and Reading Questions: I will assign the reading (on the order of 10 pages) for the next class through the blackboard web system within a couple hours of completion of a class. Doing this reading as preparation for the class is critical to being able to follow the material in the class and allows the lecture to reinforce your reading. Following the lecture, the problem sets then further the learning, and the weekly quiz provides frequent checks. In preparation for most classes, I will ask (via Blackboard) a brief reading question. There will be 30 of these questions, each graded as one point. Twenty of these points will count towards the normal point total, and up to 10 points will be extra credit to reward you for careful reading of the book. Therefore, I list 20 points as in the normal points and 10 points of extra credit for the total 30 points of reading questions.

<u>Laboratories:</u> As a part of this course, we will carry out a set laboratory experiments that will help you to see physical examples of the concepts you are learning in class. The laboratory experiments are graded on participation in the laboratory, your laboratory notebook, completion of pre- and post-lab work (when applicable), and brief written laboratory reports assigned as a part of the post-lab work. Specific grading procedures are described in the first laboratory session and through a handout at that time.

<u>Grading:</u> Tentative Grade Scale (If you get at least 90%, you are guaranteed an "A". I may elect to set the grade cutoffs lower, but we will not set them higher.) I will not be using +/- grading.

Grade	<u>Percentage</u>
A	90 %
В	80 %
С	70 %
D	60 %

Important dates:

Alaska Civil Rights Day (MLK birthday, holiday)	Monday, 21 Jan
Last day for drops (course does not appear) and 100% tuition+fee r	efund Friday, 25 Jan
Spring Break (holiday)	Monday - Friday, 11-15 Mar
Last day for withdrawals (W appears on academic record)	Friday, 29 Mar
Final Exam (10:15-12:15)	• •

Summary of Resources:

Faculty—Bill Simpson, NSF 186, 474-7235, wrsimpson@alaska.edu

Chem332 home page: log into the blackboard system: https://classes.alaska.edu/ —syllabus, sample exams and solutions, solutions to quizzes, homework solutions, email to faculty, links to other sites.

Tentative Schedule of topics (see blackboard website for detailed reading assignments):

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Wk.	Dates	Chap.	Topic	Evaluation	
1	14-18 Jan	7	Quantum Theory – Schroedinger equation	Q1 23 Jan	
2	23,25 Jan	7	Quantum Postulates / Simple systems	Q2 28 Jan	
3	28 Jan-1 Feb	7	Particle in the box and harmonic oscillator	Q3 4 Jan	
4	4-8 Feb	7,8	Review and rotation / hydrogen atom	E1 6 Feb	
5	11-15 Feb	8	Hydrogen atom, multi-electron atoms	Q4 18 Feb	
6	18-22 Feb	8,9	Multi-electron atoms, diatomic bonding	Q5 25 Feb	
7	24 Feb-1 Mar	9	MO theory, polyatomic bonding	Q6 4 Mar	
8	4-8 Mar	9, 10	Review and molecular interactions	E2 6 Mar	
	11-15 Mar		Spring Break – No classes		
9	18-22 Mar		Molecular symmetry (Handouts)	Q7 25 Mar	
10	25-29 Mar	11	Rotation-vibration of diatomics	Q8 1 Apr	
11	1-5 Apr	11	Rotation-vibration of polyatomics,	Q9 8 Apr	
			electronic spectra		
12	8-12 Apr	11	Review and computational chemistry	E3 19 Apr	
13	15-17 Apr	12	Probability / Boltzmann distribution	Q10 22 Apr	
14	22-26 Apr	12	Statistical mechanics	Q11 29 Apr	
15	29 Apr		Review for final		

Tentative schedule of laboratories (see blackboard website for details / handouts):

Lab#	Date	Topic		
1	22 Jan	Introduction to lab, safety, and digital notebook skills		
2	29 Jan	Computational Chemistry: Introduction		
3	5 Feb	Particle in a box: Spectra of long conjugated molecules		
4	12 Feb	The Spectrum of a One-Electron Atom: Hydrogen		
5	19 Feb	Spectra of multi-electron atoms: Helium (long report)		
6	26 Feb	Comp. Chemistry: Electronic potential energy curves		
7	5 Mar	Electronic structure calculations: Conjugated pi systems		
		Spring Break – No Lab		
8	19 Mar	The Spectrum of Conjugated pi systems		
9	26 Mar	The Rotation-Vibration Spectra of diatomic molecules (long report)		
10	2 Apr	Polyatomic spectroscopy: CHCl₃ vibrations		
11	9 Apr	Iodine Electronic spectroscopy and analysis		
12	16 Apr	Fluorescence of polyatomic aromatic hydrocarbons		
13	23 Apr	Computational Chemistry: Statistical mechanics		