

Instructor	Prof. William R. Simpson
Office	NSF 186 and IARC 335, Office: 907 474-7235 Lab: 907 474-2436
Email	wrsimpson@alaska.edu
Class meeting	Monday, Wednesday, and Friday 10:30 - 11:30 AM, REIC 165 (if CDC COVID-precaution guidelines can be met, via Zoom otherwise – link in Blackboard)
Laboratory Section	Tuesday, 11:30 – 2:30 PM, REIC 245 (sometimes in Chemistry computer lab, REIC 172, also via Zoom if CDC COVID-precautions not met)
Office hours	Mon, Fri 11:30AM—12:30PM, Tu 10:30-11:30AM, and by appointment
Text	“Physical Chemistry” by Atkins, de Paula, and Keeler 11 th edition Handouts for laboratory section

Course Description (from catalog): 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)

Course Goal: 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.

Learning Outcomes: In this semester, you will study quantum mechanics with applications in atomic and molecular structure, spectroscopy, and statistical mechanics. At the end of the course, successful students will have gained new mathematical methods for solving chemical problems and have learned advanced concepts that allow them to understand chemical behavior from a quantum mechanical basis. Successful students will be able to:

- Describe quantum mechanical behavior, how it differs from classical mechanics, and use concepts such as wavefunctions, operators, predict observables, and understand the uncertainty principle.
- Apply quantum mechanics to the problems of translational, rotational, and vibrational motion and the electronic structure of atoms and molecules including atomic and molecular orbital theory.
- Use quantum mechanics concepts including symmetry (group theory) to interpret atomic spectra, and molecular rotational, vibrational, and electronic spectra and extract molecular structural information such as molecular shapes and bond angles and lengths.
- Understand the statistical mechanics basis of thermodynamics and predict populations of energy levels as a function of temperature (Boltzmann distribution) and relate these statistical mechanical results to classical thermodynamics.

See the schedule for specific topics to be covered.

Course structure: The course follows your text in the order described in the attached schedule of topics. 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 and video modules will be assigned to be watched before the next class. **You must watch the lecture and read book material before class to be prepared to work on problems in class.** During class time, we will work on problems related to the assigned material, I will answer any questions, and in some cases, if there are difficult concepts, I may work problems. Watching the video and reading

the book **before** the lectures will be important for you to participate in classes. The Monday (typically) classes will review answers from the quizzes. These weekly 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 experimental examples of the concepts you learn in class.

Grading Structure (points): 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 (8 at 5 points each)	40
Weekly answer to in-class question (14*3pts = 42 pts, but two of these points will be extra credit)	40
Pre-class video questions	20
Laboratory	150
Total	650
Extra credit: Reading questions (10 of these XC points + 2 XC points from in-class questions)	+12

Exams: The exams will be given during class and will be one hour in length. Exams will be in-person. If you are not in Fairbanks due to COVID, we will determine a proctoring method – contact me. 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**.

Make up exams: 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*.

Student Protections and Services: 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 type 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/

Disability Services: 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 uaf-disabilityservices@alaska.edu, 474-5655 or by TTY at 474-1827 or <http://www.uaf.edu/disability>.

Incomplete Grade Policy: The letter "I" (Incomplete) is a temporary grade used to indicate that the student has satisfactorily completed (C or better) the majority of work in a course but for

personal reasons beyond the student's control, such as sickness, has not been able to complete the course during the regular semester. Negligence or indifference are not acceptable reasons for an "I" grade.

COVID-19 statement: Students should keep up to date on the University's policies, practices, and mandates related to COVID-19 by regularly checking this website:

<https://sites.google.com/alaska.edu/coronavirus/uaf/uafstudents?authuser=0>

Further, students are expected to adhere to the university's policies, practices, and mandates and are subject to disciplinary actions if they do not comply.

Syllabus Revision: 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.

Homework: Physical chemistry is a hard class. I see three ways that the class is hard: 1) Mechanically: It can be hard to calculate the correct answer because of algebra complexities or unit conversions. Some of your homework problems are designed to hone these skills. A solid mathematics background also helps. 2) Conceptually: You will have to find the right technique to solve a problem or identify the formula appropriate for the problem. 3) Theoretically: Many of the central concepts of physical chemistry reappear throughout the class. Therefore, seeing parallels between what at first appear to be different problems assists you in mastering the material of physical chemistry. This is the true power of physical chemistry. For example, in general chemistry, you learned about equilibrium constants and also about vapor pressures of gases. In this class, you will discover that both processes are described by the same theory.

Homework and weekly quizzes are critical aspects of learning these three parts of physical chemistry. 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). I expect that most of these homework problems will be worked during the class sessions. If a problem is not worked, its solution (along with all problems) will be posted. In this case, please 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 generally be given before 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 precede all Monday classes except on the Monday following the week of an hour exam, which will be skipped (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: Working in groups is an excellent way to reinforce knowledge and help each other. Both the student who gets help and gives help get benefits. You could work with others in a video chat session, via telephone, or other methods. I'd like to hear what works for you and am very open to enhancing the main class via your successful methods.

Video/Reading Assignments and Video Questions: I will assign the video and reading (on the order of five pages) for the next class through the blackboard web system within a couple hours of completion of a class. Watching the video and 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. During-class problems then further the learning, and the weekly quiz provides frequent checks. In preparation for most classes, I will ask (via Blackboard) a brief video 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.

Laboratories: As a part of this course, we will carry out a set laboratory experiments that will help you to see experimental examples of the concepts you are learning in class. The laboratory experiments are graded on participation in the laboratory meeting (via Zoom during the normally scheduled time or in-person if possible), completion of pre- and post-lab work, 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.

Grading: 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 %
B	80 %
C	70 %
D	60 %

Important dates:

Alaska Civil Rights Day (MLK birthday, holiday)Monday, 18 Jan
 Last day for drops (course does not appear) and 100% tuition+fee refundFriday, 22 Jan
 Spring Break (holiday) Monday - Friday, 8-12 Mar
 Last day for withdrawals (W appears on academic record)Monday, 22 Apr
 Final Exam (10:45AM-1:15PM)..... Thursday, 29 Apr

Summary of Resources:

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

Chem332 web 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):

Wk.	Dates	Chap.	Topic	Evaluation
1	11-15 Jan	7	Quantum Theory – Schroedinger equation	Q1 20 Jan*
2	20,22 Jan	7	Quantum Postulates / Simple systems	Q2 25 Jan
3	25-29 Jan	7	Particle in the box and harmonic oscillator	Q3 1 Feb
4	1-5 Feb	7,8	Review and harmonic oscillator / rotation, H atom	E1 3 Feb
5	8-12 Feb	8	Hydrogen atom / multi-electron atoms	Q4 15 Feb
6	15-19 Feb	8	Atomic (electronic) spectroscopy	Q5 22 Feb
7	22-26 Feb	8,9	Multi electron atoms, diatomic bonding, MO theory	Q6 1 Mar
8	1-5 Mar	9	Review and Polyatomics	E2 3 Mar
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9	15-19 Mar	10	Molecular symmetry	Q7 22 Mar
10	22-26 Mar	11	Rotation-vibration of diatomics	Q8 29 Mar
11	29 Mar- 2Apr	11	Rotation-vibration of polyatomics, electronic spectra	Q9 5 Apr
12	5-9 Apr	11	Review and computational chemistry	E3 7 Apr
13	12-16 Apr	13	Probability / Boltzmann distribution	Q10 19 Apr
14	19-23 Apr	13	Statistical mechanics	Q11 26 Apr
15	26 Apr		Review for final	

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

Lab#	Date	Topic
1	19 Jan	Introduction to lab, safety, and digital notebook skills
2	26 Jan	Computational Chemistry: Introduction
3	2 Feb	Particle in a box: Spectra of long conjugated molecules
4	9 Feb	The Spectrum of a One-Electron Atom: Hydrogen
5	16 Feb	Spectra of multi-electron atoms: Helium
6	23 Feb	Comp. Chemistry: Electronic potential energy curves
7	2 Mar	Electronic structure calculations: Conjugated pi systems
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8	16 Mar	The Spectrum of Conjugated pi systems
9	23 Mar	The Rotation-Vibration Spectra of diatomic molecules
10	30 Mar	Polyatomic spectroscopy: CHCl ₃ vibrations
11	6 Apr	Iodine Electronic spectroscopy and analysis
12	13 Apr	Fluorescence of polyatomic aromatic hydrocarbons
13	20 Apr	Computational Chemistry: Statistical mechanics