Chemistry 432 - Physical Chemistry II
Course Syllabus
Spring 2019

1. Instructor: Dr. David L. Freeman
   Phone: x 4-5093
   Office: 474C Beaupre
   Office Hours: MWF 11 or by appointment
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2. Scheduling: MWF 10, 105 Beaupre

3. Text:
   (a) Thomas Engel, "Quantum Chemistry and Spectroscopy," Pearson, Benjamin Cummings, 2013, Third Edition
   (b) Thomas Engel and Philip Reid, "Thermodynamics, Statistical Thermodynamics and Kinetics," Pearson, Benjamin Cummings, 2013, Third Edition

4. Prerequisites: CHM 192 or CHM 112, MTH 142, PHY 112 or 204, CHM 431. Knowledge of the material in these courses will be assumed.

5. Course requirements:

(a)	Weekly quizzes (every Friday) The lowest 2 numerical scores will be dropped in determining grades.	300
(b)	Final exam (Friday, May 3, 8:00-11:00 AM)	200
(c)	Total	500

   Grades will be determined on a curve. Incompletes will be given only for valid medical reasons. Quizzes cannot be made up. Please note that if the University is closed on a Friday for snow or any other reason, the weekly quiz will be given on the next class day the University is open.

6. Illness Due to Flu
   The nation is experiencing widespread influenza-like illness. If any of us develop flu-like symptoms, we are being advised to stay home until the fever has subsided for 24 hours. So, if you exhibit such symptoms, please do not come to class. Notify me at 874-5093 or freeman@chm.uri.edu of your status, and we will communicate through the medium we have established for the class. We will work together to ensure that course instruction and work is completed for the semester.

   The Centers for Disease Control and Prevention have posted simple methods to avoid transmission of illness. These include: covering your mouth and nose with tissue when coughing or sneezing; frequent washing or sanitizing your hands; avoiding touching your eyes, nose, and mouth; and staying home when you are sick. For more information please view www.cdc.gov/flu or flu.gov . URI Health Services web page, www.health.uri.edu , will carry advice and local updates.

7. Course Goals:

   As can be made clear by examining your textbooks, physical chemistry is subdivided into a number of distinct topics. Last semester you learned the laws of thermodynamics which govern the behavior of chemical systems at equilibrium. This semester we will extend our understanding of the laws of chemistry to the microscopic and non-equilibrium domains.

   One of the major cultural and intellectual achievements of the twentieth century has been the discovery of the laws of quantum mechanics. Although a complete introduction to quantum theory requires one year, we will be able to *understand some of the principles of quantum mechanics and the implications of the theory to chemistry.* This is our first course goal. Closely allied with a discussion of the laws of quantum theory is *to understand elementary atomic and molecular electronic structure.* This second course goal is a consequence of quantum mechanics. Another consequence of quantum theory has been the field of spectroscopy. *Understanding how spectroscopy is used to determine the microscopic properties of molecules* is our third course goal.

   Although much insight can be obtained from the microscopic laws of nature, it is important to learn the connection between the microscopic laws and the thermodynamics you learned last semester. We meet this goal by studying statistical mechanics, which rigorously connects microscopic information with macroscopic thermodynamics. If time permits, we also connect microscopic and macroscopic information using kinetic theory, which is approximate but insightful. Kinetic theory is also useful in meeting the last goal of CHM 432. Our final course goal is to leave the equilibrium domain *to begin to obtain an understanding of non-equilibrium phenomena.* We shall study non-equilibrium phenomena within the context of the kinetic theory of matter and the study of chemical reaction kinetics.

8. The CHM 432 Web page:

   In this course all problem sets, problem set solutions and quiz solutions are to be distributed on the course web page. No paper copies of the problem sets are to be distributed. The URL of our course web page is
   http://www.chm.uri.edu/courses/?chm432&1 . It is strongly suggested that you link to our web page to obtain the first problem set as soon as possible.

   It is expected that for most of you, success in this course will require some level of help beyond classroom instruction. Because some of you may find it difficult to come to the scheduled office hours, we have installed as part of our course web pages, a page that can be used to submit questions. Questions are submitted by anyone in the class by filling out a form on the web page, and answers are distributed either to the entire class or only to the person asking the question. If the entire class is to receive a copy of the question and answer, the question is treated as anonymous; i.e. the person who asks the question is never identified. In fact, it is possible to submit a question so that even the instructor does not know who submitted the question. Anonymous questions and responses by the instructor are distributed to your email addresses listed on ecampus and Sakai. With ordinary electronic mail, there is a private correspondence between the student and instructor. By using the web page, the entire class has an opportunity to learn from the questions submitted.

   The use of the web page does not preclude personal interaction between any of you and the course instructor. Dr. Freeman has regular office hours, and you are all encouraged to make use of these hours. Alternate meeting times can be arranged by appointment. Additionally, you can contact Dr. Freeman by e-mail or telephone. The e-mail address and phone number for Dr. Freeman is given on the first page of this syllabus.

   Any student in CHM 432 can submit questions and comments to Dr. Freeman. Submission of such comments or questions must be made using the WWW home page for this course. The address (URL) of our home page is
   http://www.chm.uri.edu/courses/?chm432&1 . To submit a question to the list, you must click on the highlighted text that says "submit a question to the CHM 432 list." As an example of how to use the list, suppose a student in our class, Ms. Benzene Ring, wonders, "What are the units of wavefunctions?" (If you don't know what this means, don't worry. You will understand the question early in the semester). To obtain an answer to her question, Ms. Ring links her web browser (e.g. Chrome, Firefox, Safari or Microsoft Internet Explorer) to http://www.chm.uri.edu/courses/?chm432&1, and she then clicks on the text linking her to the page for questions (i.e. the highlighted text that says "submit a question to the CHM 432 list"). Ms. Ring then enters her e-mail address in the appropriate box and specifies whether she wants her question to be answered to the entire CHM 431 class or to her alone. Ms. Ring then types in the large box
   `What are the units of wavefunctions?`
   Ms. Ring then clicks the "send" button. Ms. Ring's question is received by Dr. Free-

man. Dr. Freeman then sends an e-mail message to the whole list that might be

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Subject:  wavefunction units
The question is:  What are the units of wavefunctions?
Answer:  In one dimension, the units are 1/\sqrt{length}.
In three dimensions the units are 1/\sqrt{volume}.
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Now Ms. Ring and the entire class have an answer to her question. In the answer \sqrt{} stands for a square root, and this notation is discussed below.

If the answer to the question can be sent to the entire list, the answer will not indicate who asked the question. If Ms Ring wants to ask the question with full anonymity so that even Dr. Freeman has no idea who asked the question, the e-mail portion of the form can be left blank. Of course, if the e-mail section of the form is blank, the answer must be sent to the list and not just to the sender.

Because many questions may contain mathematical formulas, we need a notation to communicate the special symbols used in the course. To avoid confusion, it is most useful if we agree on the same set of symbols. The symbols that follow are taken from a language called LaTeX. LaTeX is a language that is frequently used to prepare scientific documents, and LaTeX can be used to translate special symbols into simple text characters. By learning LaTeX notation, you will learn a widely used method to communicate mathematical symbols via e-mail. The instructor plans to use these symbols in answering your questions, and it is asked that you use the same symbols in posing questions. The most important symbols are the following:

(a) Greek letters are represented by \ followed by the name of the letter. For example α is typed `\alpha`, β is typed `\beta`, and so on. A Greek letter is made upper case by making the first letter of its name upper case. For example, the letter Δ is typed `\Delta`.

(b) Subscripts are represented by _{} where the brackets contain the subscripts. For example, μ_{ij} is typed `\mu_{ij}`.

(c) Superscripts are represented by ^ {} where the brackets contain the superscripts. For example, β^{12} is typed `\beta^ {12}`.

(d) Infinity (∞), is typed `\infty`.

(e) The integral sign $\int$ is typed `\int`. The limits on a definite integral are included by introducing subscripts and superscripts. As an example $\int_0^\infty e^{-x^2} dx$ is typed `\int_{0}^ {\infty} e^ {-x^ {2}} dx`.

(f) The partial derivative symbol ∂ is typed `\partial`.

(g) The summation sign $\sum$ is typed `\sum`. The lower and upper limits of summation are included as subscripts and superscripts. As an example $\sum_{n=0}^{\infty} 1/n^2$ is typed `\sum_{n=0}^ {\infty} 1/n^ {2}`.

(h) Square roots $\sqrt{a+b}$ are typed `\sqrt{a+b}`.

(i) The arrow in chemical reactions $\rightarrow$ is typed `--->`. For example $C + O_2 \rightarrow CO_2$ is typed `C + O_{2} ---> CO_{2}`.

Let us now look at another example of a question submitted using the web. In this case, Ms. Ring has a question requiring an equation. This might be a real question. If you don't understand the context, don't worry. You will understand the details of the question later in the course. Suppose Ms. Ring wants to ask

"In calculating an expectation value, the expression is

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi^* \hat{A} \psi dx$$

For calculating the expectation value of the momentum, what operator do we use for A?"

To submit the question, Ms. Ring uses her web browser to attach to http://www.chm.uri.edu/courses/?chm432&1, clicks on the line that says, "submit a question to the CHM 432 list," and then Ms. Ring enters the information requested by the form. If Ms. Ring wishes to remain anonymous, Ms. Ring leaves the e-mail box blank. Ms. Ring then types into the large box

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In calculating an expectation value, the expression is
< A > = \int_{-\infty}^ {\infty} \psi^ * A \ psi dx.
For calculating the expectation value of the momentum, what operator do we
use for A?
```

and clicks on the submit button. Ms. Ring's question is received by Dr. Freeman. The answer will be sent either to Ms. Ring alone, or preferably to the entire class if the appropriate box is checked. Dr. Freeman might reply

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Subject:  Momentum Operator
The question is:In calculating an expectation value, the expression is
< A > = \int_{-\infty}^ {\infty} \psi^ * A \ psi dx.
For calculating the expectation value of the momentum, what operator do we
use for A?

The answer is:  A=p=hbar/i d/dx
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9. Course outline[1]:

Topic	Book Chapter
1. Review of Classical Mechanics and the Quantum Nature of Matter	(a) 1, 6.3
2. The Schrödinger Equation	(a) 2.2-2.5
3. The Postulates of Quantum Mechanics	(a) 3
4. Simple Quantum Systems	(a) 4, 5.5
5. Vibrational and Rotational Motion	(a) 7
6. Vibrational and Rotational Spectroscopy of Diatomic Molecules	(a) 8.1, 8.3-8.6, 8.8
7. The Hydrogen Atom	(a) 9
8. Many-electron Atoms	(a) 10.1-10.4
9. Atomic Spectroscopy	(a) 11.1-11.4
10. Chemical Bonding	(a) 12, 13.8
11. Molecular Electronic Spectroscopy	(a) 14.1-14.4, 14.6-14.8
12. Statistical Mechanics	Handout
13. Kinetic Theory (time permitting)	(b) 16
14. Chemical Kinetics	(b) 18
15. Final Exam	Comprehensive

[1] (a) = "Quantum Chemistry and Spectrocscopy," (b) = "Thermodynamics, Statistical Thermodynamics and Kinetics"