1. Instructor: Dr. David L. Freeman  
   Phone: x 4-5093  
   Office: 474C Beaupre  
   Office Hours: MWF 11 or by appointment  
   e-mail: freeman@chm.uri.edu

2. Scheduling: MWF 10, 105 Beaupre

3. Text:

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 5, 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 in an approximate way by studying kinetic theory. Kinetic theory not only gives an ideal-gas molecular description to some of the macroscopic laws of nature, but 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 automatically to everyone who has
submitted their e-mail address to the instructor. 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.

To receive copies of the submitted questions and the answers to the questions, you must
submit your e-mail address. The method of submission uses our web page. Go to our
home page (http://www.chm.uri.edu/courses/?chm432&1) and click on “Subscribe to
the CHM 432 list.” On the resulting form, enter your e-mail address, click on the small
“subscribe” button and then click on the submit button. You can also use this form
to unsubscribe from the list in case you drop CHM 432.

Any student in CHM 432 can submit questions and comments to Dr. Freeman. Sub-
mmission 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. Firefox or Microsoft In-
ternet 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. Freeman. Dr. Freeman then sends an e-mail message to the whole list that might be

Subject: wavefunction units
The question is: What are the units of wavefunctions?
Answer: In one dimension, the units are $1/\sqrt{\text{length}}$.
In three dimensions the units are $1/\sqrt{\text{volume}}$.

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 $\backslash$ followed by the name of the letter. For example $\alpha$ is typed $\backslash alpha$, $\beta$ is typed $\backslash beta$, and so on. A Greek letter is made upper case by making the first letter of its name upper case. For example, the letter $\Delta$ is typed $\backslash Delta$.

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

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

(d) Infinity ($\infty$), is typed $\backslash infty$.

(e) The integral sign $\int$ is typed $\backslash int$. 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 $\backslash int_{\{0\}}^{\{infty\}} e^{-x^2} \{\{2\}\} dx$.

(f) The partial derivative symbol $\partial$ is typed $\backslash partial$. 


(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 $\sum_{\{n=0\}}^{\infty} 1/n^2 \{2\}$.

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

(i) The arrow in chemical reactions $\rightarrow$ is typed $\rightarrow$. For example C+O$_2$ $\rightarrow$ CO$_2$ is typed C + O$_2$ $\rightarrow$ 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

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

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:

In calculating an expectation value, the expression is

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

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:

Subject: Momentum Operator

The question is: In calculating an expectation value, the expression is

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

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

The answer is: $A = p = h\bar{\imath} / d/dx$

Remember, your first task is to subscribe to the CHM 432 list either by e-mail or filling out the form on our web pages. You can then send questions and comments to Dr.
Freeman using your web browser starting at the URL http://www.chm.uri.edu/courses/?chm432&1.

9. Course outline¹:

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¹(a) = “Quantum Chemistry and Spectroscopy,” (b) = “Thermodynamics, Statistical Thermodynamics and Kinetics”