CHEMISTRY 3060[1]
Physical Chemistry
FALL 2009

Instructor: David Farrelly, ML153, 797-1608, email: david.farrelly@usu.edu (please put CHEM3060 somewhere in the subject header.) Or, preferred, use CourseMail.

Time and Location: MWF 9:30 a.m. - 10:20 a.m., LIB 405.

Office Hours: Drop in anytime is OK if I have time.

Monday	10:30 - 12:30
Thursday	10:30 - 12:30
Friday	1:30 - 2:20.

Textbook & Material: *Physical Chemistry* (any recent edn.) by I. N. Levine; Chapters 1 - 16.

WebCT: A web page will be available through Blackboard. I will deposit notes there and post Bulletins. You can also send email using CourseMail though this site.

Grading: There will be weekly quizzes, graded problem sets, and three in-class exams: two midterm exams and a final. Midterm dates will be decided in class. See below for details of how these will operate. They will count toward the grade as follows.

Quizzes	10%
Homeworks	30%
Midterms	30%
Final	30%.

Final grades will be assigned based on the actual distribution of scores obtained by the class rather than being based on predetermined cutoffs. However, normally an overall score greater than 80% will be an A or A-. The problems sets and exams are designed to be challenging.

Mathematics: Physical chemistry requires an ability to use mathematical techniques; in CHEM3060 this includes multivariate calculus, differential equations and linear algebra. It is strongly suggested - but not required - that you obtain a book with a title similar to: *"Mathematics for the Physical Sciences."* Examples include *Mathematical Methods for Scientists and Engineers* by McQuarrie (∼$86) and *Applied Mathematics for Physical Chemistry* by Barrante (∼$28). McQuarrie's book is excellent and much more thorough than Barrante but it is also more expensive.

[1] In accordance with the Americans with Disabilities Act, reasonable accomodation will be provided for all persons with disabilities in order to ensure equal participation in this course.

1 Assignments and Quizzes

1.1 Quizzes

There will be a 15 min quiz every Friday (with occasional exceptions) which will start at around 9:30 a.m. and will conclude at around 9:45 a.m.. The first few minutes of class will be for questions, if any. Here are the rules:

1. Quizzes will consist of five short questions each of which will be graded 0 or 1. The material will *usually* be based on the previous 3 or 4 lectures but any material covered to that point in the semester - including homework assignments and prior quizzes - may be tested.
2. Quizzes must be worked in Examination Blue Books.
3. If you miss a quiz for any reason then make arrangements with me to make it up at my discretion.

1.2 Homework Assignments

Homework assignments will usually be given every Wednesday. They will be due on the Friday of the following week. Here are the rules:

1. A spiral-bound notebook should be used for homework assignments.
2. What you hand in should reflect your final best attempt at a solution. It need not show all of the steps that you actually took (e.g., wrong turns) to reach that solution. However, key steps in the solution should be clearly shown together with short explanations of what you did, e.g., *"next integrate over r to ..."*. That is, the solution you hand in should be similar to what you would expect to see in a solutions manual.
3. You will lose points if your answers don't contain brief statements explaining what you are doing. An unbroken stream of correct mathematics is not enough!
4. It is suggested that you first work the problems out on scrap paper and then transcribe your final attempt into your notebook.
5. Each problem will be worth 5 points unless otherwise stated and each assignment will be worth 50 points.
6. Each assignment should be started on a new page and be clearly labelled and dated.
7. Only one side of the paper should be used.
8. Assignments should be done in ink. Mistakes should be neatly crossed out or whited out. Assignments done in **pencil** will **NOT** be accepted.

9. Problems should be clearly numbered and different problems should be separated by two or three blank lines.

10. Illegible or untidy work will not be graded. Too small writing and/or homeworks done on loose-leaf paper will never be graded. I may refuse to grade your homework and ask you to redo it neatly.

11. Incomplete or incorrect solutions may still receive full credit if the approach was sensible.

12. If you cannot complete a problem, just state that and leave a blank to finish the problem later.

I will make exceptions to any of the rules regarding quizzes and assignments but please try to follow the rules as closely as possible.

2 Office Hours

You can ask anything about lectures, homeworks, quizzes etc. If you don't understand something but don't know what to ask then that is acceptable too. You are welcome to come individually or with other members of the class in a small group. Dont wait for regular office hours if you have a question. But please understand if, on occasion, I can't deal with you then and there.

3 Physical Chemistry Learning Objectives

1. Apply the basic concepts of calculus to concepts in chemistry.

2. Manipulate the gas laws to describe real and ideal gas behavior.

3. Discuss the Three Laws of Thermodynamics and their development.

4. Use the Maxwell equations and other thermodynamic relations to compute thermodynamic quantities from thermodynamic data tables.

5. Be able to derive relationships between thermodynamic quantities.

6. Interpret phase diagrams and discuss phase equilibria in terms of chemical potential.

7. Explain the origin ofK_{eq} and its relation to fugacity and activity; apply these concepts to ideal and real solutions of electrolytes and non-electrolytes and to colligative properties.

8. Apply the principles of electrochemistry to conductance, voltaic, and electrolytic systems.

9. Provide a physical basis for Debye-Huckel theory.

10. List the methods for arriving at a plausible mechanism and/or rate law based on kinetic information.
11. Apply the steady-state hypothesis to obtain rate equations.
12. Explain the basic principles of photochemical and radiation-chemical reactions.
13. **Explain the origin of quantization and the break down of classical mechanics.**
14. **Solve the Schrödinger equation for some simple systems.**
15. **Use operator notation for eigenvalue equations.**
16. **Use the quantum mechanical results for the particle in a box, the simple harmonic oscillator, and the rigid rotor to interpret the dynamics and spectra of molecular systems.**
17. **Calculate expectation values of operators and probabilities of measured values.**
18. **Sketch molecular orbitals and electron probability distributions for simple systems.**
19. **Write down wavefuntions of correct spin symmetry for many-particle systems.**
20. **Derive term symbols and classify molecules according to symmetry.**
21. **Explain how radiation interacts with matter using mathematical equations and symmetry.**
22. **Derive selection rules from symmetry considerations.**
23. **Explain how perturbations lift degeneracy.**
24. **Explain how lasers work.**
25. **Compare and contrast spectroscopic techniques.**
26. **Explain what a partition function is and how it can be derived in principle from an equation of state and how it relates to the equilibrium constant.**
27. **Estimate the contributions of molecular translation, rotation, vibration, and electronic excitation to thermodynamic functions.**
28. **Derive the ideal gas law from quantum mechanics.**
29. **Explain how quasi-equilibrium states can exist and how this leads to transition state theory.**

30. **Explain the origin of intermolecular forces and be able to make intelligent speculations on which predominate in any given substance.**

More general goals of the physical chemistry program are that the student is able to:

1. Demonstrate competency in written and oral communication including using mathematics.
2. Relate the microscopic and macroscopic properties of matter to each other.
3. Apply thermodynamic, kinetic and quantum methods and concepts to all areas of chemistry and biochemistry.
4. Explain what the main areas of research in physical chemistry are and why research is being done in these areas.
5. Make either oral or written criticisms of research articles in physical chemistry.
6. Design real or gedanken experiments or simulations to test hypotheses.

Assessment

In order to gauge the effectiveness of the course, several different methods of Gain Score Analysis will be employed. A gain score is a measurement of how much a students capability has (hopefully) increased from the beginning of a class and the completion of the course. One measurement is the comparison of the performance on weekly quizzes and to the performance on the midterm exams. Another measurement is how the midterm exam scores compare to the comprehensive final exam grade. Throughout the semester, embedded questions will be presented. These kind of questions emphasize the above-mentioned Learning Objectives and help us assess the overall quality of the course.