

FAIRLEIGH DICKINSON UNIVERSITY

Metropolitan Campus

SYLLABUS for PHYSICAL CHEMISTRY I (FALL 2007)

Course Title: Physical Chemistry I Credits: 3
Course Number: CHEM 3241.51
Day: Wednesday
Time: 5:25 pm - 8.00 pm Room: TBA
Instructor: Dr. Arthur R. Murphy
Office: DH 4413 Office Hours: M W F 11:00 AM – Noon and by appointment
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Required Text: Physical Chemistry (5th Edition) by Ira Levine ISBN 0-07-231808-2

Catalog Description for Physical Chemistry I and II.

The principles of physical chemistry from the molecular and microscopic aspects: kinetic theory, quantum mechanics, spectroscopic studies and statistical concepts; thermodynamics, chemical and phase equilibria, electrolytes and electrochemistry..

Policies and Procedures:

- 1) All cell phones, beepers, and pagers must be turned off during lecture.
- 2) Students are expected to arrive for class on-time so as not to disrupt a lecture in progress.
- 3) All homework assignments will have a due date on them: Typically a student will have two weeks in which to complete an assignment. Late homework assignments will not be accepted.
- 4) Last Day for dropping the course with a grade of "W" is November 4th.

Grading Policy

Final Grade = 50 % Exam Grades + 50 % Homework Grades

Introduction:

Chemists, and other scientists are interested in the properties and behavior of chemical systems, and these systems show patterns and regularities that can be analyzed using quantitative physical principles. Physical Chemistry provides us with a powerful organizational tool to study phenomena encountered in many areas of chemistry, biology, and physics. Schematically:

Physical Chemistry Principles (both the macro and micro worlds and the relationships between them)	Explanations, Insights ===== >	Phenomena encountered in Organic Chemistry, Inorganic Chemistry, Analytical Chemistry, Biochemistry, and other fields.
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Physical Chemistry is one of the corner stones of science, and it is composed of many sub-areas among which are:

- 1) Classical and non-classical Thermodynamics (macroscopic approach) including phase chemical and phase equilibria.
- 2) Statistical Mechanics (microscopic approach to thermo)
- 3) Quantum Chemistry (atomic and molecular structure)
- 4) Spectroscopy (Ex. Vibr., Rot., electronic, NMR etc.)
- 5) Kinetics (Reaction rates, mechanisms)
- 6) Electrochemistry
- 7) Biophysical Chemistry
- 8) Computational Chemistry

Expectations:

- 1) In order to be successful in this course, students are expected to be proficient in the use of calculus. A good background in the scientific applications of microcomputers is also very desirable. However, use of pertinent software will be reviewed as needed.
- 2) Students will be expected to become familiar with the primary Physical Chemical literature. This includes current books, current Journals, monographs, and Web sites devoted to Physical Chemistry.
- 3) To be successful in this Physical Chemistry course, students should do as many problems in the textbook as possible. In addition to Physical Chemistry textbooks, P. Chem. problem solving books exist, and a short list of those most likely to be of use to students is given in the "Literature" section of this syllabus.

Course objectives and outcomes:

Objective 1: To learn macroscopic and microscopic aspects of ideal and real gases.

Outcome 1.1: Students will review and understand simple gas laws and the ideal equation of state.

Outcome 1.2: Students should understand and be able to apply a variety of Equations of State, such as the Virial, Redlich-Kwong, and Peng-Robinson equations, for the analysis of real gas behavior.

Outcome 1.3: Students should know and be able to apply various aspects of the Kinetic Theory of Gases among which are collision frequencies, the Maxwell Boltzmann Distribution of speeds, effusion processes, mean free paths, and the Boltzmann distribution law.

Objective 2: To learn those aspects of Classical Equilibrium Thermodynamics that are useful in other areas of Chemistry such as Inorganic Chemistry, Biochemistry, etc.

Outcome 2.1: Students should have reviewed the mathematics associated with thermodynamics: Line integrals, partial derivatives, and the use of Mathcad to facilitate calculations.

Outcome 2.2: Students should understand key concepts such as empirical and thermodynamic temperature scales, heat, work, reversible and irreversible process, and state functions (E , H , S , G).

Outcome 2.3: *Students should understand the zeroth, first, second, and third laws of thermodynamics.*

Outcome 2.3 *Students should understand how thermodynamics is applied to material equilibrium. They should know*

- (i) *Standard Thermodynamic Functions of Reactions: Standard States, calorimetry, temperature dependence of reaction enthalpies, how to use thermodynamic tables, and know how to estimate of thermodynamic properties.*
- (ii) *The thermodynamics of ideal gas mixtures and how the chemical potential is used.*

Outcome 2.5 *Students should understand how thermodynamics is applied to phase equilibria.*

- (i) *one component phase equilibria should be understood.*
- (ii) *Select multicomponent phase equilibria should be understood.*

Outcome 2.4 *If time permits, ideal and real solutions will be investigated . Otherwise this material will be saved for Physical Chemistry II.*

- (i) *Students should understand the difference between ideal and real solutions.*
- (ii) *Students should understand activities, activity coefficients, and fugacity and there applications.*

ADDITIONAL “OUTCOMES”

Students who successfully complete this course should have a good background for pursuing Physical Chemistry II, as well as courses in other sciences that require knowledge of Physical Chemistry.

TEACHING METHODOLOGIES / ACTIVITIES

- 1) The fundamental method of transmitting material to the students is by means of traditional lectures.
- 2) Web resources will be used where appropriate.
3. Students will receive instructions on how to use Mathcad. Knowledge of this software should greatly help students with their homework assignments.
- 4) In order to assess student’s understanding of the material, major hourly exams as well as homework assignments will be given.

COURSE OUTLINE

TENTATIVE LECTURE SCHEDULE

Week #	Date	Topic
1	8/29/07	Gases (Chapter #1 Sec 1.5) + Real Gases Chapter #8
2	9/5/07	(Chapter #8 continued) + Kinetic Molecular Theory of Gases Chapter #15)
3	9/12/07	(Chapter # 15 Continued)
4	9/19/07	Chapter #1 (Thermodynamics) + Chapter #2 (the 1st Law of Thermo.
5	9/26/07	Exam #1
6	10/3/07	The First Law of Thermodynamics (Chapter #2 + The Second Law of Thermodynamics (Chapter #3))
7	10/10/07	The 2nd Law of Thermodynamics (Chapter #3) +
8	10/17/07	Material Equilibrium (Chapter #4) + Standard Thermo Functions of Reaction.(Chapter #5)
9	10/24/07	Reaction equilibrium in ideal gas mixtures. (Chapter #6)
10	10/31/07	Exam #2
11	11/7/07	Solutions (Chapter #9)
12	11/14/07	Nonideal solutions (Chapter #10) +
13	11/21/07	Recess
14	11/28/07	One component Phase equilibrium (Chapter # 7) Multicomponent phase equilibrium Chapter #12
15	12/5/07	TBA
16	12/12/07	Final Exam

The Physical Chemistry Literature – a First Look.

- I. Books containing many solved problems are:
 - A. Adamson, Arthur W., Understanding Physical Chemistry, Benjamin-Cummings 3rd Ed., 1980. This paperback has been placed on reserve in the library.
 - B. Labowitz, Leonard, Arents, J., Physical Chemistry Problems and Solutions. Academic Press, 1969. This paperback has been placed on reserve in the library.
 - C. Metz, Clyde, Schaum's Outline of Physical Chemistry, 2nd edition, McGraw-Hill, 1988. (paperback).
 - D. Fogiel, M., Ogden, J. The Physical Chemistry Problem Solver: a complete solution guide to any textbook. Research and Education Assn. 1994 (paperback.)
- II. Textbooks
 - A. Silbey, R., Alberty, R. , Physical Chemistry, 3rd Edition, Wiley, 2000 This book

has some good problems as well as a nice discussion of standard states used in Biochemistry.

- B. McQuarrie, D., Simon, J., Physical Chemistry: A molecular approach, University Science Books, 1997. This is an excellent advanced text. High quality problems too! Earlier printings of this book omitted discussions of the thermodynamics of solutions. The later printing included this information.
- C. Atkins, Peter, Physical Chemistry 6th Edition, Freeman, 1998. I prefer some of the earlier editions of this textbook. Graphics are good and there is a large selection of problems at the end of each chapter.
- D. Noogle, J., Physical Chemistry 2nd Edition, Scott Foresmen and Co. This is a very good P. Chem textbook. Lots of good problems.
- E. Laidler, K., Meiser, J., Sanctuary, B. Physical Chemistry 4th Edition, Houghton Mifflin Co, 2003. This is a good introductory text. Beginning students should find the material accessible. Many end of the chapter problems.
- F. Lesk, A. , Physical Chemistry, Prentice Hall, 1982. This is another textbook that deserved more recognition than it received. Many of the subjects were given a fresh look.
- G. Barrow, G. Physical Chemistry 6th edition, McGraw-Hill 1996. This book has numerous problems, and the beginning student may find the presentation style very accessible.

III. Useful Math textbooks

- A. Boas, M. Mathematical Methods in the Physical Sciences 2nd Edition, Wiley, 1983. This is a excellently written book. Crisp, clear descriptions and lots of problems. Highly recommended.
- B. Barrante, James, Applied Mathermatics for Physical Chemistry, Prentice Hall, 1998. Very concise. Beginners may find it of interest. I've donated my copy to the library.

IV. Physical Chemistry and Computers

- A. Noogle, J. , Physical Chemistry Using MathCad, Pine Creek Pub., 1997. This book provides a nice introduction to computer applications in many areas of Physical Chemistry. I only wish that more advanced applications were included.

V. Physical Chemistry and the Web

- A. Throughout this course, URL's will be given to interesting P. Chem. Sites. For now, I mention only a few of these.
 - (i) www.monmouth.edu/~tzielins/mathcad/
This site is a repository for many documents that use MathCad in Physical Chemistry.
 - (ii) <http://science.widener.edu/~svanbram/mathcad.html> This is another site

containing applications of MathCad to P. Chem. Scroll down to the hyper link “Mathcad for Physical Chemistry at WSU” and following links. Most folder names should be self explanatory.

- (iii) Thermodynamic Data:
<http://webbook.nist.gov/chemistry/> This is a wonderful site for obtaining a great deal of current thermodynamic data. The National Institute of Science and Technology is the successor to the National Bureau of Standard.
- B. Physical and Thermodynamic Properties of the elements
<http://webelements.com>. One of my favorite chemistry web sites.

VI. Physical Chemistry Journals

- A. The ACS Journal of Physical Chemistry A and The Journal of Physical Chemistry B are available on-line from FDU’s network. In the past, this Journal was not divided into “A” and “B” parts.
- B. The Journal of Chemical Physics. Older issues of this journal are available at FDU’s library. For current issues, consult libraries at other institutions.
- C. Physical Chemistry related e-journals available at FDU are
 - (i) Theochemica Acta
 - (ii) Electrochemica Acta
 - (iii) Electrochemistry Communications
 - (iv) Chemical Physics
 - (v) Chemical Physics Letters