

CHEM 460/544: Chemical Thermodynamics Syllabus – Fall 2007

Abstract: Thermodynamics consists of a set of empirically derived postulates concerning the thermal behavior of materials. It provides a powerful framework for inter-relating material properties and for understanding physical and chemical equilibria and transformations. Most thermodynamic data is derived from experiment, but such data is enriched and extended by molecular models of thermal behavior -- the domain of statistical mechanics or “molecular” thermodynamics.

CHEM 453/544 provides a survey of formal aspects of thermodynamics and its use in practical situations. Much of the material covered will be similar to that introduced in general physical chemistry courses: the underlying principles of thermodynamics and application of these principles to problems of reaction and phase equilibria in pure phases and solutions. However, these topics will be covered in greater depth and a higher level of sophistication will be expected from students. In addition to classical thermodynamics, some elementary statistical mechanics will be introduced in order to help provide insight into the molecular origins of bulk behavior.

Schedule: Chem 460/544 302 Willard MWF 1:15 – 2:15 PM
Instructor: Will Noid 528 Chemistry Building wnoid@chem.psu.edu

Office Hours: No fixed hours. Drop in at any time or e-mail for an appointment.

Required Texts:

1. *Thermodynamics and an Introduction to Thermostatistics*. H.B. Callen (Wiley 2nd ed 1985).
2. *Introduction to Statistical Mechanics*. T.L. Hill (Dover reprint 1987).

Recommended Text:

1. *Statistical Mechanics: Principles and Selected Applications*. T.L. Hill (Dover reprint 1987).

Course Web: I will try to post HW assignments and solutions on the course website: <http://courses.chem.psu.edu/chem544>

Prerequisites: Although the course will begin with the basics, it will be assumed that students have already learned the material covered in an undergraduate physical chemistry course similar to Chem 451. (Chem 451 spends the majority of a semester treating the fundamentals of thermodynamics.) Chem 460/544 will quickly cover the fundamentals of thermodynamics with greater rigor and sophistication than in standard undergraduate physical chemistry courses. Time permitting, the course will also provide a somewhat rigorous introduction to the fundamental principles of statistical mechanics. A *working* knowledge of elementary calculus will be assumed. In particular, application of the “chain rule” for differentiation of multivariable functions will frequently be important for the text and assignments. I suspect that comprehension of the basics reviewed in appendix A in Callen will be invaluable.

Class Format & Assignments: Class will primarily be spent introducing/reviewing concepts and expanding on reading material. The goal will be to cover roughly a chapter of Callen each week through the end of the material on thermodynamics. Homework will be assigned for each

chapter on roughly a weekly basis. Students are *strongly encouraged* to keep up with the course by reviewing lecture notes and reading the text presently being covered. Because the objective of the class is for students to master the fundamental concepts underlying thermodynamics and statistical mechanics, students will be required to explicitly formulate/outline the approach for solving each problem. Typically, full credit for a problem will require not only correctly outlining the problem, but also arriving at the correct answer. However, considerable partial credit will be earned by explicitly formulating the correct approach for solving the problem. Extra credit may be earned by presenting homework problems for the class. Additional extra credit opportunities will be provided for students enrolled in Chem 460.

Grading: Grades will be based on 3 exams (25% each) and on class participation and assignments (25%).

Exam Dates: Exams are tentatively scheduled for the following dates and times:

- Exam I: Thursday, October 11, 6:30-8:30 p.m.
- Exam II: Thursday, November 15, 6:30-8:30 p.m.
- Exam III: During Finals Week (date and time to be announced)

If you have a conflict with one of these times, *please let me know as soon as possible*. The format may vary among open-book, closed-book, and take-home exams. I am presently leaning towards open-book closed-note exams.

Academic Honesty: Collaboration in learning the course material and on homework assignments is encouraged. However, I also strongly encourage you to consider HW assignments as an opportunity to gauge your comprehension of the course material and to make sure that you master the concepts related to each HW set. Furthermore, all examinations must be taken individually. Any instance of giving or receiving aid on an examination will be viewed as a serious offense, which may result in a failing grade for the course and/or referral to the University disciplinary system.

All Penn State policies regarding ethics and honorable behavior apply to this course (see links below for policy statements). Academic integrity is the pursuit of scholarly activity free from fraud and deception and is an educational objective of this institution. All University policies regarding academic integrity apply to this course. Academic dishonesty includes, but is not limited to, cheating, plagiarizing, fabricating of information or citations, facilitating acts of academic dishonesty by others, having unauthorized possession of examinations, submitting work of another person or work previously used without informing the instructor, or tampering with the academic work of other students. For any material or ideas obtained from other sources, such as the text or things you see on the web, in the library, etc., a source reference must be given. Direct quotes from any source must be identified as such. All exam answers must be your own, and you must not provide any assistance to other students during exams. Any instances of academic dishonesty WILL be pursued under the University (<http://www.psu.edu/ufs/policies/>) and Eberly College of Science (<http://www.science.psu.edu/academic/Integrity/index.html>) regulations concerning academic integrity.