

CHEM 6471

CHEMICAL THERMODYNAMICS AND KINETICS

Class Meetings

9:35 – 10:55 am, Tuesday and Thursday, August 21 – December 6, Room 1201A MS&E Bldg.

Holidays: Tuesday, October 9 (mid-term recess) and Thursday, November 22 (Thanksgiving).

No class on Tuesday and Thursday, August 28 and 30 due to instructor travel.

Office hours: Wednesday, 9:30 –11:00 am or by appointment with the following exceptions:

- (i) no office hours during the week of August 27–31
- (ii) office hours on Tuesday, 11:30 am – 1:00 pm during the week of October 22–26

Textbooks

Molecular Thermodynamics by D.A McQuarrie and J.D. Simon, University Science Books, Sausalito, CA, 1999, ISBN 1-891389-05-X.

Problems and Solutions Manual to accompany the above textbook, by H. Cox and C.A McQuarrie, University Science Books, Sausalito, CA, 1999, ISBN 1-891389-07-6 (*optional*).

Reaction Kinetics by M.J. Pilling and P.W. Seakins, Oxford University Press, Oxford, UK, 1995, ISBN 0-19-855527-X; reprinted 1996 (with corrections), 1997 (with corrections), 1999, 2001, 2002, 2003, 2005.

Prerequisite

Two semesters of undergraduate physical chemistry or equivalent

Description

This course covers the laws of classical thermodynamics and some of their chemical applications. It also covers basic statistical thermodynamics and chemical kinetics. The level of the course is meant to be intermediate between an undergraduate physical chemistry course and more advanced graduate courses in physical chemistry and related disciplines.

Grading Policies

Three exams will be given during the semester. The exams will be administered during normal lecture periods. The exam dates (all Thursdays) are September 20, October 25, and November 29. For students taking the final exam (see below) each exam will count 20% of the course grade.

Homework will be assigned periodically and will be graded. Students are encouraged to collaborate on homework assignments, but each student should turn in their own homework *in their own writing (or word processing)*. For students taking the final exam (see below), graded homework will count 15% of the course grade.

A three-hour final exam will be given at the date and time established by normal Georgia Tech procedures (tentatively scheduled for Friday, December 14 at 8:00 am). The final exam will count 25% of the course grade. Students who receive $\geq 80.0\%$ of the possible points on the exams and homework will receive an A grade in the course and will not have to take the final exam.

Changes in Exam Grades

Changes in exam grades must be requested within *one week* of the class period that the graded exam is returned to students; exam grades become “carved in stone” after this one week period.

Student Honor Code

Students are expected to adhere to the Georgia Tech honor code (see <http://honor.gatech.edu>).

Electronic Distribution of Course Material

Information will be provided during the early part of the semester.

Syllabus

The schedule given below may be overly optimistic and, therefore, is subject to "tweaking" as the semester progresses. However, the three exam dates are "carved in granite".

The Properties of Gases

Lectures: August 21, 23

Reading: McQuarrie & Simon, Chapter 2 and Math Chapters A, C, & D; Supplementary Material I

Review of Energy Levels of Atoms and Molecules

Lectures: No lectures on August 28, 30 (use extra time to work on Homework Set 1)

Reading: McQuarrie & Simon, Chapter 1

Elementary Probability Theory, the Boltzmann Distribution, and Partition Functions

Lectures: September 4, 6, 11, 13

Reading: McQuarrie & Simon, Chapters 3 & 4 and Math Chapters B & E

Catch-up and Review

Lecture: September 18

Reading: None

Exam No. 1, September 20

The First Law of Thermodynamics

Lectures: September 25, 27 and October 2

Reading: McQuarrie & Simon, Chapter 5

Entropy and the Second and Third Laws of Thermodynamics

Lectures: October 4, 11, 16

Reading: McQuarrie & Simon, Chapters 6 & 7

Helmholtz and Gibbs Energies

Lectures: October 18, 20

Reading: McQuarrie & Simon, Chapter 8

Catch-up and Review

Lecture: October 23

Reading: None

Exam No. 2, October 25

ADDED: Phase Equilibria (Reading: McQuarrie & Simon, Chapter 9, 1-2 lectures)

Chemical Equilibrium

Lectures: October 30, November 1, 6

Reading: McQuarrie & Simon, Chapter 12

Introduction to Chemical Kinetics

Lectures: November 8, 13

Reading: Pilling & Seakins, Chapters 0, 1, & 2

Theories of Bimolecular Reactions

Lectures: November 15, 20

Reading: Pilling & Seakins, Chapter 3

Catch-up and Review

Lecture: November 27

Reading: None

Exam No. 3, November 29

Unimolecular and Association Reactions

Lectures: December 4, 6

Reading: Pilling & Seakins, Chapter 5

Final Exam, Friday, December 14 at 8:00 am (tentative)