

Ch21c Spring 2008

web site:<http://www.its.caltech.edu/~ch21c/index.html>
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Requirements: 8 problem sets 50%
1 first midterm 25%
1 second midterm 25%
Collaboration on problem sets allowed, but no direct copying
NO USE OF SOLUTION MANUAL FOR CURRENT TEXTBOOKS
(REQUIRED OR RECOMMENDED)
NO USE OF SOLUTIONS FOR PRIOR YEAR PROBLEM SETS OR EXAMS

Late Policy: 5% per day, no credit after one week.
If the late policy is abused, the penalty will be increased to 10%
per day.

This class assumes that you are continuing from Ch21a and b, and that you are familiar with basic quantum mechanics, spectroscopy, and elements of statistical mechanics (energy, entropy, and partition functions).

Required Text: Silbey, Alberty, Bawendi, Physical Chemistry (Wiley, 2004)
p-chem text from the Other Institute of Technology

Maczek, Statistical Thermodynamics (Oxford University Press, 1998)

Recommended Texts:
Denbigh, Chemical Equilibrium (Cambridge, 1981)
Excellent though older text

Houston: Chemical Kinetics and Reaction Dynamics, (McGraw-Hill, 2001).
good standard graduate/advanced undergraduate text for kinetic theory, kinetics, and reaction dynamics

References:

Thermodynamics and Statistical Mechanics

There are many many texts on thermodynamics and statistical mechanics. Here are a few at the undergraduate level.

- Smith, Basic Chemical Thermodynamics, 5th ed. (Oxford, 2004)
concise elementary intro
- Mandl, Statistical Physics, 2nd ed. (Wiley, 1988)
Good coverage of statistical derivation of thermodynamics
- Fermi, Thermodynamics (Dover, 1936)
classic text by one of the Masters of physics; short but deep
- McQuarrie, Molecular Thermodynamics (University Science Books, 1999); also McQuarrie and Simon, Physical Chemistry (University Science Books, 1997).
a good p-chem text
- Widom, Statistical Mechanics (Cambridge University Press, 2002)
Light reading on modern topics by a giant in the field
- Bowley and Sanchez, Introductory Statistical Mechanics, Oxford University Press, 1999).
Another good statistical mechanics text, but notation is different

Kinetics and Reaction Dynamics

There are many good books on kinetics, relatively few good ones on dynamics. Many kinetics only books (Johnston, Preston and Schwarz, Pilling and Seakins) are quite good. For this class, I also recommend

- Houston: Chemical Kinetics and Reaction Dynamics, (McGraw-Hill, 2001).
*good standard graduate/advanced undergraduate text
for kinetic theory, kinetics, and reaction dynamics*
- Steinfeld, Francisco and Hase, Chemical Kinetics and Dynamics (Prentice Hall, 1999).
excellent kinetics, transition state theory, and statistical rate theory

Ch21c SYLLABUS

Equilibrium Systems and Gases (Weeks 1-2)

I. Introduction to Equilibrium Systems

II. Kinetic Theory of Gases

Classical Thermodynamics

(Weeks 2-6)

III. First Law of Thermodynamics

Differential Forms

First Law of Thermodynamics

Enthalpy

IV. Second Law of Thermodynamics

Entropy

Legendre Transformations, Maxwell Relations

V. Free Energy and Chemical Potential

Applications

VI. Phase Transitions

Phase diagrams

Clayperon Equation, Clausius-Clayperon Equation, Gibbs phase rule

VII. Third Law of Thermodynamics

VIII. Mixtures

IX. Critical Phenomena

Van der Waals Equation of State

Critical points

X. Advanced Topics

Activities; electrochemistry

Fluctuations, correlations, and fluctuation-dissipation theorem

Water

Polymers

Statistical Thermodynamics

I. Statistical Thermodynamics of Independent Particles

(Week 7)

(continued from ch21b)

Review of thermodynamic Laws

Third Law and Residual Entropy (Blake notes)

A,G,H in terms of partition function q

II. Chemical potential μ

Chemical equilibrium

III. Quantum Statistics

Reactions

(Weeks 7-10)

I. Reaction Kinetics

First and second order kinetics, atmospheric chemistry

II. Transition State Theory

III. Physical Kinetics: Diffusion

IV. Solution Phase Reactions

V. Molecular Collisions

Classical mechanics of two body collisions

VI. Reaction Dynamics

VII. Photochemistry