This is an introductory graduate course in physical chemistry focused on the thermodynamics of chemical processes, with an emphasis on fundamental principles and practical applications. The course begins with a review of undergraduate thermodynamics from a graduate-level perspective. A deeper understanding of chemical thermodynamics is developed systematically, using simple model systems as examples and building up to the description of more complex systems. Applications discussed in the second half of the semester include the thermodynamics of self-assembly and irreversible processes of relevance to the biological structures and nano-devices, as well as the effects of solute-solvent interactions on chemical reactions. It is hoped that this course will be of use to graduate students with a variety of backgrounds and interests, acting as a bridge to higher level graduate courses in physical chemistry or as a stand-alone out-of-area course. The only pre-requisite for this course is undergraduate physical chemistry.
Chemical Thermodynamics

Fundamentals of Chemical Thermodynamics (6-7 weeks)
- Basic concepts and formal postulates
- Thermodynamic Temperature
- Fundamental Equation
- Entropy representation
- The chemical potential
- Euler and Gibbs-Duhem equations
- Legendre transformations (leading to H, G, A, etc.)
- Quasistatic processes, reversible work and spontaneity
- Inequalities associated with the 2nd Law
- Maxwell Relations

Selected Applications of Chemical Thermodynamics (3-4 weeks)
- Phase transitions, Trouton’s rule and Clausius-Clapeyron equation
- Experimental measurement of Entropy
- Chemical reaction thermodynamics (in the gas phase)
- Self-assembling chemical systems
- Nano-machines and irreversible processes

Introduction to Statistical Thermodynamics (2-3 weeks)
- Boltzmann factor
- Partition functions, q and Q
- Relationship between Q and thermodynamic functions
- Boltzmann Entropy and Other ensembles

The Effects Intermolecular Interactions on Chemical Equilibria (2-3 weeks)
- Non-ideal gases - the second virial coefficient
- Chemical reactions in non-ideal gases
- Liquid perturbation theory - the van der Waals equation
- Generalized van der Waals theory of liquids
- Equations of state of pure fluids and mixtures
- Solvent effects on chemical equilibria
- Ionic solutions - Dielectric continuum approximation
Homework, Examinations and Final

Several homework assignments will be given during the semester (between 6 and 8 assignments). Each will consist of a set of short questions requiring relatively simple calculations. These are designed to reinforce the key concepts of thermodynamics rather than demonstrate the derivation of complex multi-step results.

Two in-class examinations will be give during the semester. These will consist of short questions related to the homework problems and class discussion. The first exam will cover Fundamentals of Chemical Thermodynamics. The second exam will cover the Applications of Chemical Thermodynamics and the Foundations of Statistical Thermodynamics.

The take-home final will resemble an extended homework assignment pertaining to The Effects Intermolecular Interactions on Chemical Equilibria.

Approximate point breakdown:

- Homework 100 points
- Exam I 100 points
- Exam II 100 points
- Final 100 points
- Total 400 points
## CHM 679 - Fall 2006
### Reserve Book List

<table>
<thead>
<tr>
<th>Title</th>
<th>Author(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermodynamics and an Introduction to Thermostatistics</td>
<td>H. B. Callen</td>
</tr>
<tr>
<td>Molecular Driving Forces (^{(a)})</td>
<td>K. A. Dill &amp; S. Bromberg</td>
</tr>
<tr>
<td>Modern Thermodynamics. From Heat Engines to Dissipative Structures</td>
<td>D. Kondepudi &amp; I. Prigogine</td>
</tr>
<tr>
<td>Thermodynamics</td>
<td>Honig</td>
</tr>
<tr>
<td>An Introduction to Statistical Thermodynamics</td>
<td>T. L. Hill</td>
</tr>
<tr>
<td>Statistical Mechanics. A Concise Introduction for Chemists</td>
<td>B. Widom</td>
</tr>
<tr>
<td>Physical Chemistry</td>
<td>Moore</td>
</tr>
<tr>
<td>Physical Chemistry</td>
<td>Castellan</td>
</tr>
<tr>
<td>Physical Chemistry</td>
<td>Atkins</td>
</tr>
<tr>
<td>Gases, Liquids and Solids</td>
<td>Tabor</td>
</tr>
<tr>
<td>States of Matter</td>
<td>Goldstein</td>
</tr>
<tr>
<td>Statistical Mechanics</td>
<td>McQuarrie</td>
</tr>
<tr>
<td>Solvation Thermodynamics</td>
<td>Ben-Naim</td>
</tr>
<tr>
<td>Solvents and Solvent Effects in Organic Chemistry</td>
<td>Reichardt</td>
</tr>
<tr>
<td>Molecular Theory of Gases and Liquids</td>
<td>Hirschfelder, Curtis &amp; Bird</td>
</tr>
<tr>
<td>Computer Simulation of Liquids</td>
<td>Allen &amp; Tildesley</td>
</tr>
</tbody>
</table>

\(^{(a)}\) This book is on reserve in the Potter Engineering Library; call number 536.7 D58m