Chemistry 711: Chemical Thermodynamics

Last update: for Fall 2015
Instructor: Andrew Cooksy (/faculty/Cooksy/)
email: acooksy@mail.sdsu.edu (mailto:acooksy@mail.sdsu.edu)
office/lab: CSL-310,307,312; tel: 594-5571

Tentative course calendar (course_calendar.php)

Syllabus

Lecture Meetings: Tue, Thu 5:00-6:15pm, SSW-2512
Office Hours: Tue/Thu 3:00-4:00pm, CSL-310. These office hours are shared with another class, so please be patient if you come by and I'm with other students.
Textbook: Andrew Cooksy, *Physical Chemistry: Thermodynamics, Statistical Mechanics, and Kinetics*. We will not be using the online homework available with this text, so you are welcome to look for used copies. This is a textbook for part of the undergraduate physical chemistry course, but covers enough advanced topics that I think it will suffice as the basic text for the course. The lectures may occasionally extend to material beyond the scope of the textbook. We will *not* be using the last two chapters of the book that cover chemical kinetics or the introductory Chapter 1. We should get to most of the rest, which we will cover in class in the same order as in the book.
Solutions to End-of-Chapter problems: Worked solutions are available in the free solutions manual from Pearson (http://www.pearsonhighered.com/chemistryresources/) (click on the "Solutions Manual (PDF)" link for our book). Please conserve paper: store this electronically and refrain from printing out the entire manual.

General Idea

This course is intended to benefit chemistry graduate students in all areas, as well as students in other departments with interests in the fundamentals of energy distribution and dynamics in molecular systems. A complete undergraduate, calculus-based p-chem course (the equivalent of our CHEM 410A and 410B) is expected. You're welcome to contact me if you want to ask about the course content or what would be suitable preparation for the course. The emphasis should be on the principles of statistical mechanics and thermodynamics common to all applications of chemistry, so students are encouraged to bring issues from their own research or other interests to the attention of the instructor for discussion (the sooner the better).

Student learning objectives:

At the conclusion of the course, the student should be able to:

- Define thermodynamic properties such as entropy, temperature, and free energy.
- Describe qualitatively the distribution of energy in any molecular system, and how it changes with temperature.
- Calculate basic dynamical properties of systems, such as mean free path and average collision frequency, relating these to observable properties.
- Derive and use algebraic expressions for the thermodynamics of specific systems.

• Predict trends in the energy distributions, thermodynamic properties, and energy level populations of molecular systems.

Course material

Chemical statistical mechanics and thermodynamics, which together provide our best theory for how energy is distributed in ordinary matter and exchanged during chemical processes.

General Plan:

Statistical Mechanics
  Entropy and temperature
  Partition functions
  Mass and energy transport
Chemical Thermodynamics
  The laws of thermodynamics
  Phase transitions and solutions
  Chemical reactions
  Your Application Here

Prerequisite Math

You should be comfortable with algebra and the simple derivatives and integrals (especially of the functions ax^n, e^{ax}, and $\sin(ax)$ or $\cos(ax)$). See Chapter A in the book for a review of relevant math and physics. There is some calculus that I don't expect everyone to remember that we will review in class. If you're still not too confident or have any questions, just come and see me and we can review during office hours.

Grading criteria

Grading Scheme

- homework: 10%
- three exams: 15% each (drop lowest score)
- computational project: 15%
- paper presentation: 20%
- final: 25%

The grading scale is fairly lenient:
A 80-100%
B 65-80%
C 50-65%
It is graduate physical chemistry, after all.

Exam Dates for Fall 2015

- exam 1: Thu Sep 24
- exam 2: Thu Oct 22
- exam 3: Thu Nov 19
- final exam: Thu Dec 17 3:30pm-5:30pm

Computational Project and Paper Presentation

I may modify these instructions, but here is the tentative plan. Suggested modifications are welcome.

Paper Presentation

Chem 711 students will present a 20-minute PowerPoint or chalkboard talk to the class, based primarily on one or two papers. Each presentation will be critiqued by students and the instructor, and comments will be consolidated by the instructor.

Students are graded based on both their presentation and on their participation in the evaluations of their classmates. You should email me your topic and relevant reference(s) as soon as possible, and we should have the assignments finalized no later than Friday, October 23. **The talks will be presented outside of class, at additional times to be determined** between Nov. 12 and Dec 11. Please be prepared to attend these presentations over the course of two or three additional meetings. Once we know when everyone can be available, I will assign the dates and times of the talks to individual speakers at random and post them.

Computer project

It is fairly straightforward now to use electronic structure programs such as Gaussian 09 to predict thermodynamic properties of chemical systems, but it helps to have some guidance. Students will select a single chemical reaction and carry out calculations to predict ΔH, ΔG, and other properties of the system. Results will be presented in a short but *professional quality* report (say, 2-3 pages). All work must be completed and reports submitted by email no later than Monday, Dec 14 at midnight.

Students with Disabilities

If you are a student with a disability and believe you will need accommodations for this class, it is your responsibility to contact Student Disability Services at (619) 594-6473. To avoid any delay in the receipt of your accommodations, you should contact Student Disability Services as soon as possible. Please note that accommodations are not retroactive, and that accommodations based upon disability cannot be provided until you have presented your instructor with an accommodation letter from Student Disability Services. Your cooperation is appreciated.