Chemistry 711: Chemical Thermodynamics — Course Syllabus

Fall 2021, Tues & Thurs 5:00 – 6:15, AH-3150

Instructor Dr. David Pullman, CSL–301, 619–594–5573, dpullman@sdsu.edu

Office Hours TBD

Textbook *Molecular Thermodynamicscs*, D.A. McQuarrie ans J.D. Simon, ISBN: 978-1891389054

Prerequisites Chemistry 410B or equivalent

Catalog Description Chemical Thermodynamics and an Introduction to Statictical Thermodynamics

Course Structure The lectures will roughly follow the text, with additional examples drawn from the chemical literature and perhaps from research in SDSU's Chem&Biochem Department. Some lectures will be devoted to tutorials in the use of computer software; these lectures will be held in the departmental computer lab, GMCS-245 (Note: you do *not* need to purchase any software since it will be available on the departmental computers). During the last week of classes, each student will give a ~25 minute presentation discussing a literature article they have selected.

Grading

Exam I	22% (*tentatively* the week of September 27)
Exam II	22% (*tentatively* the week of October 25)
Final Exam	31% (Thursday December 16, 2021, 3:30 – 5:30)
Final Project	25% (presented Dec. 7 and Dec. 9)

- No makeup exams will be given.
- The grading scale is:

A	80-100%
B	65-80%
C	50%-65%

+/– grading will be used

- The final project consists of selecting (in consultation with the instructor) a paper from the research literature in which classical or statistical thermodynamics plays an important role and preparing and presenting a ~25 minute talk to the class in which you discuss and critically evaluate the article. 80% of your grade for the project will be based on your presentation, while 20% will be based on your participation in asking questions during the other student presentations.

Topics We will cover topics from all or parts of the following chapters (and perhaps others, as needed) in the text:

Chap 1 The Energy Levels of Atoms and Molecules
Chap 2 The Properties of Gases
Chap 3 The Boltzmann Factor and Partition Functions
Chap 4 Partition Functions and Ideal Gases
Chap 5 The First Law of Thermodynamics
Chap 6 Entropy and the Second Law of Thermodynamics
Chap 7 Entropy and the Third Law of Thermodynamics
Chap 8 Helmholtz and Gibbs Energies
Chap 9 Phase Equilibria
Chap 10 Solutions I: Liquid-Liquid Solutions
Chap 12 Chemical Equilibrium

Student Learning Outcomes

Upon completing Chem 711, students will be able to:

1. Understand and articulate the basic principles of Chemical Thermodynamics
2. Understand and articulate the basic principles of Statistical Thermodynamics
3. Describe the fundamental thermodynamic properties of molecular system in terms of the energy levels of the molecules
4. Calculate thermodynamic quantities for chemical reactions
5. Perform thermodynamic calculations and simulations using Excel, Igor, and Gaussian
6. Evaluate the literature regarding thermodynamic measurements of complex reaction systems

Problem Sets

There will usually be one problem set per chapter. Problem sets will ***not*** be graded; you do not need to hand them in. You can download them from the Canvas website for the class. **As in any technical class, doing the problem sets is of the utmost importance to learning the material and doing well on exams**.

Add/Drop Procedure

The add/drop deadline is Sept. 3, 2021 at 7:59 PM. For details, see http://arweb.sdsu.edu/es/registrar/schedule_adjustment.html

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 Ability Success Center at (619) 594-6473. To avoid any delay in the receipt of your accommodations, you should contact Student Ability Success Center as soon as possible. Please note that accommodations are not retroactive, and that I cannot provide accommodations based upon disability until I have received an accommodation letter from Student Ability Success Center. Your cooperation is appreciated.