

Chemical Thermodynamics & Dynamics

CHEM 217, 3 credits

Reference Books & Notes

- Class notes are available online and can also be downloaded.
- Physical Chemistry by Atkins, 6th edition, Oxford University Press, 1998.
- Physical Chemistry by Alberty and Silbey, 3rd edition, Wiley, 2001.

CATALOG DESCRIPTION

Covers the basic principles of chemical thermodynamics and chemical dynamics. Mathematical machinery of the laws of thermodynamics. Heat, work, and energy. First, second, and third laws of thermodynamics. Thermodynamics of chemical reactions. Thermodynamics of solutions. Transport properties: diffusion, viscosity, ion transport, thermal conductivity. Chemical kinetics. Collision theory. Activated complex theory.

COURSE OBJECTIVES

- Provide students with a lasting and solid understanding of thermodynamics.
- Effectively teach fundamental concepts such as entropy, enthalpy, fugacity, free energy, chemical potential.
- Teach students how to set up and solve thermodynamics problems.
- Provide opportunities for students to become proficient using computer tools for solving problems.
- Expose students to the molecular basis for chemical reactions.
- Give students a working knowledge of the chemical kinetics literature.
- Train students how to use reaction mechanisms as a basis for mathematical kinetics models.
- Show students how and why reaction rates can be sensitive to the reaction medium.
- Teach students the role of kinetics and catalysis in the atmosphere.
- Understand and use transport equations like the diffusion equation, laws of Fick, Fourier, and Newton.

Course Outcomes

- Apply the laws of thermodynamics to chemical processes.
- Calculate differences in thermodynamic properties using equations of state, charts and tables, and computer resources.
- Explain the microscopic, fundamental basis of thermodynamics.
- Interpret thermodynamic data.
- Understand the concept of temperature dependence of the reaction rates.
- Develop a reaction rate expression for a given reaction mechanism.
- Propose a mechanism consistent with an experimentally determined rate law.
- Use experimental data to estimate parameters in a rate law.
- Assess whether numerical values of kinetics parameters are chemically meaningful and consistent with theory.
- Rationalize reaction medium effects in terms of fundamental chemical or physical principles.
- Understand and apply simple molecular reaction dynamics calculations.
- Account of the reaction rates (in gas phase or solution) in terms of the Collision theory.
- Account of the reaction rates in terms of the Transition complex theory.
- Identify strategies for and issues involved in stratosphere pollution.

Topics to be covered and downloaded

- Introduction and the zeroth law
- First Law
- Thermochemistry
- Carnot theorem & Second law; uncompensated heat
- Third law
- Thermodynamic potentials
- Free energy and Maxwell relations
- Open systems and mixing
- Chemical Equilibrium
- Thermodynamics of solutions
- Kinetic theory and transport phenomena
- Introduction to reaction kinetics; Arrhenius equation; integrated rate laws
- Elementary and complex reactions
- Consecutive and reversible reactions; relaxation methods
- Unimolecular reactions; Lindemann-Hinshelwood mechanism
- Reaction Mechanisms

- Steady-state and equilibrium approximations
- Potential energy surface; Activation energy
- Collision theory
- Activated Complex Theory
- Atmospheric chemical cycles

Assessment

- Two quizzes (30% higher grade, 20% lower grade) and a final exam (50%).
- End of term course evaluation provides student self-assessment of outcomes.

Policy

Students are expected to attend all lectures. Attendance will be taken periodically in class. Students must attend the lecture in the section for which they are registered. Absence from quizzes and/or the final is not permitted. If a student is prevented from taking a quiz for reasons beyond his or her control, he or she should notify their professor as soon as possible. If the reason is judged to be acceptable, the professor will work out a grading scheme for the final grade. Any student who, for any reason, misses the two quizzes, will be asked to withdraw from the course. No Make-up Quizzes will be given. In the case of absence from the final examination with valid reasons, a student is entitled to a make-up final exam, after the approval of the professor and the Arts and Sciences Dean's office.