

COURSE DESCRIPTION: This course provides a mathematically rigorous fundamental understanding of how heat, work, and entropy are related to chemical transformations (chemical reactions and physical changes in state) through the laws of thermodynamics and concepts related to statistical mechanics. The course will also provide the basic principles of chemical kinetics and its relation to transition state theory.

CREDITS: This is a 3 credit hour course

PREREQUISITES: MATH 273 or 283 with a C or better; PHYSICS 202 with a C or better.

CLASS SCHEDULE: M,W,F from 10:10am to 11:00am in Fulmer 438

TEXTBOOK: "Physical Chemistry: A Molecular Approach" by D. A. McQuarrie and J. D. Simon (required)

SUPPLEMENTARY MATERIAL: "Applied Mathematics for Physical Chemistry" J. A. Barrante (recommended)

COURSE WEBSITE: Classroom materials will be uploaded to the web and placed in a Dropbox folder. The URL for the class website and Dropbox folder are given below:

http://stochastic4.chem.wsu.edu/brozikgroup/Course_Information.html
https://www.dropbox.com/sh/empzf8c32leovtc/AADBSZtEf_Jf7NOVOnJOosxPa?dl=0

STAFF / OFFICE HOURS:

Professor James A. Brozik, Department of Chemistry / Materials Science and Engineering
Office: Fulmer 123
Phone: 5-3746
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Office Hours: W,F 11:10am to 12:00am; Room 438 (Starting August 28th)

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Office Hours: T,Th 1:00pm to 2pm (or by appointment); Fulmer 402 (Starting August 27th)

STUDENT LEARNING OBJECTIVES: At the end of the course student should be able to:

1. Understand and apply the principles of thermodynamics to quantitatively relate work, heat, internal energy, entropy, enthalpy, Gibbs free energy, Helmholtz free energy, equations of state, the state of the system(s), and chemical potential to chemical transformations and chemical equilibrium.
2. Understand and apply rudimentary statistical mechanics principles to quantitatively relate work, heat, internal energy, entropy, enthalpy, Gibbs free energy, Helmholtz free energy, equations of state, the state of the system(s), and chemical potential to chemical transformations and chemical equilibrium.
3. Understand and apply the principles of chemical kinetics to quantitatively describe the dynamics of chemical reactions and their relation to reaction mechanisms.
4. Understand and apply transition state theory to quantitatively describe the temperature dependence of rate constants and their relation to reaction mechanisms.

ASSESSMENT:

All homework, quizzes, exams, and in-class exercises will be related to one or more of the above stated learning objectives.

EXAMS AND QUIZZES:

Exam dates are listed on the tentative schedule below. You must bring a calculator and at least 2 pencils and erasers. Unless otherwise indicated, no notes or textbooks are to be brought to the exam. If I see any signs of formulas or answers stored in calculators, on phones, or any other form of information transfer other than from your head or provided with the test, the result will be an assigned grade of zero for the exam. 2 out of 3 exams (1 hour long) with the highest grade will count toward your total exam score. A cumulative final exam (2 hours long) will also be given.

No makeup exams will be given except in the case of a university **required** activity or a serious **proven** personal emergency. A written explanation/request of the absence must be submitted to your TA and me by email **prior** to the exam date. According to Academic Regulation 80, a student will not be granted special examinations for the purpose of leaving the institution before the close of the semester. In addition Academic Regulation 78 states that during final examination week, if the scheduled arrangement results in students having three or more examinations scheduled for any one day, any of their instructors is authorized to excuse the students from the regularly scheduled examination and give a final examination to the students during the special exams time blocks.

There will be a quiz at the end of class each Friday unless the class is notified otherwise (no quiz on August 28th). All quizzes are open-note, open book. Each quiz will be worth 10 points. There will be no make-up quizzes and no exceptions to this policy. Unexcused, missed quizzes will receive a score of -10; Quizzes turned in late will receive a score of 0. Students who have completed all of the in-class quizzes will be allowed to drop one quiz at the end of the semester or have one quiz count as extra credit.

HOMEWORK:

All problems must be clearly and completely written out with words of explanation inserted where appropriate. Show all your work! Make sure you show units and significant figures. You will be graded **PRIMARILY** for your approach to the problem and demonstrated understanding of concepts. One to two problems will be selected for grading for each assignment -- the selection is random. 9 out of a potential of 12-14 assignments with the highest score will count toward your homework grade.

GRADING:

Homework	5%
Quizzes	30%
Exams	40%
<u>Final Exam</u>	<u>25%</u>
Total	100%

Grading schedule: A \geq 90; B \geq 80; C \geq 65; D \geq 50; F $<$ 50.

EMAIL POLICY:

All official WSU email communication must be sent to students' WSU email address, beginning on August 24 (the first day of fall 2015 classes). This is a University wide policy so please use your WSU email account only. The policy can be found at: <https://provost.wsu.edu/2015/08/17/wsu-email-change/>

ATTENDANCE and CLASS ETIQUETTE:

Students are responsible for obtaining and learning the material covered in lectures from which they are absent.

You are expected to participate in classroom activities in a professional manner. Private discussions with other students, passing notes, texting, reading newspapers, disruptive eating, sleeping, persistently arriving late or leaving early, use of cell phones for non-class related activities, or using the internet for non-class related activities constitute inappropriate classroom behavior. If you demonstrate such behavior you will be verbally warned in class to cease. If you persist in disruptive or distracting behavior, formal action, in accordance with WSU policy, will be taken.

It is OK to use your smart device(s) to record lectures (audio or video) and to look up material related to the lecture. In fact, there will be times that I ask students to do a quick search on related topics or access the class webpage.

STUDENTS WITH DISABILITIES:

Reasonable accommodations are available for students with a documented disability. If you have a disability and need accommodations to fully participate in this class, please either visit or call the Access Center (Washington Building 217; (509) 335-3417) to schedule an appointment with an Access Advisor. All accommodations MUST be approved through the Access Center. We MUST be notified of this documented disability at the beginning of the semester. For more information contact a Disability Specialist on your home campus at 509-335-3417 or <http://accesscenter.wsu.edu>, Access.Center@wsu.edu

ACADEMIC DISHONESTY:

Washington State University, a community dedicated to the advancement of knowledge, expects all students to behave in a manner consistent with its high standards of scholarship and conduct. Students are expected to uphold these standards both on and off campus and acknowledge the university's authority to take disciplinary action. The purpose of these standards and processes is to educate students and protect the welfare of the community. The standards of Conduct for Students can be found at <http://conduct.wsu.edu>.

University instructors have the authority to intervene in all situations where students are suspected of academic dishonesty. In such instances, responsible instructors retain the authority to assign grades to students considering, from an academic standpoint, the nature of the student action. Ideally, the consequences for such actions are spelled out beforehand in the syllabus. More information regarding responding to academic integrity violations can be found at: <http://conduct.wsu.edu>.

The definitions of academic dishonesty and the university process for handling complaints are available at this website: <http://www.conduct.wsu.edu>. Instructors retain the authority to assign grades to students considering, from an academic standpoint, the nature of the student action.

SAFETY AND EMERGENCY NOTIFICATION:

Washington State University is committed to enhancing the safety of the students, faculty, staff, and visitors. It is highly recommended that you review the Campus Safety Plan (<http://safetyplan.wsu.edu/>) and visit the Office of Emergency Management web site (<http://oem.wsu.edu/>) for a comprehensive listing of university policies, procedures, statistics, and information related to campus safety, emergency management, and the health and welfare of the campus community.

DISRUPTIVE CLASSROOM BEHAVIOR:

Behavior that persistently or flagrantly interferes with classroom activities is considered disruptive behavior and may be subject to disciplinary action. Such behavior inhibits other students' ability to learn and an instructor's ability to teach. A student responsible for disruptive behavior may be asked to leave class pending discussion and resolution of the problem and may be reported to the Office of Student Conduct.

Tentative Class Schedule

	Date		Topic	Reading
1	Aug	24	Introductory Remarks	
2		26	Molecular Degrees of Freedom / Basic Quantum Mechanical Concepts	Handout
3	Fri	28	“	
4		31	Properties of Gases	Chapter 16
5	Sept	2	“	
6	Fri	4	“	
		7	LABOR DAY CLASS HOLIDAY	
7		9	Partition Functions	Chapter 17
8	Fri	11	“	
9		14	“	
10		16	Partition Functions and Ideal Gases	Chapter 18
11	Fri	18	“	
12		21	“	
13		23	The First Law of Thermodynamics	Chapter 19
14	Fri	25	Exam 1: Includes Chapters 16, 17, 18	
15		28	The First Law of Thermodynamics	
16		30	“	
17	Oct	2	Entropy and the Second Law of Thermodynamics	Chapter 20
18		5	“	
19		7	“	
20	Fri	9	“	
21		12	“	
22		14	Entropy and the Third Law of Thermodynamics	Chapter 21
23	Fri	16	“	
24		19	Helmholtz and Gibbs Free Energy	Chapter 22
25		21	“	
26	Fri	23	“	
27		26	Phase Equilibrium	Chapter 23
28		28	“	
29	Fri	30	Exam 2: Includes Chapters 19, 20, 21, 22	
30	Nov	2	Phase Equilibrium	
31		4	Solution Equilibrium	Chapter 24
32	Fri	6	“	
33		9	“	
		11	VETERANS DAY (HOLIDAY)	
34	Fri	13	Chemical Equilibrium	Chapter 26
35		16	“	
36		18	“	
37	Fri	20	Chemical Kinetic / Transition State Theory	Chapter 28
		23	THANKSGIVING BREAK	
		25	THANKSGIVING BREAK	
	Fri	27	THANKSGIVING BREAK	
38		30	Chemical Kinetic / Transition State Theory	
39	Dec	2	“	
40	Fri	4	Exam 3: Includes Chapters 23, 24, 26, 28	
41		7		
42		9		
43	Fri	11		
44	Dec	18	Final Exam 8am to 10am Fulmer 438	