Physical Chemistry II
Thermodynamics, Statistical Mechanics, and Kinetics

Instructor

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Office hours: By appointment, or by chance

Time and Location

9:30–10:30 Tuesday/Thursday, 109 Pasquerilla Center

Course Description

Physical chemistry explains how things work in chemistry using concepts from physics and mathematics. Mathematical concepts from calculus and linear algebra will be used frequently, and this course will use more math than most other chemistry courses. In this course, we will discuss topics such as thermodynamics, gas laws, equations of state, chemical kinetics, equilibrium, and statistical mechanics. These topics provide insight into how the world around us works and why chemical and biological systems behave the way they do. Some of these topics will be familiar to you from your General Chemistry course, but these will be covered in more detail.

Being a scientist requires creative problem solving skills. This course will use a variety of methods to help develop these skills which will help in your professional careers. Traditional problems will be assigned on homework sets and in exams and some will be done in class. Open-ended problems will also be assigned throughout the semester.

Course Objectives

Upon successful completion of this course, students should be able to:

- Use mathematical approaches to solve chemical problems
- Identify the components of a thermodynamic system and make predictions about the system's behavior according to the laws of thermodynamics
- Solve, analyze, and interpret phase equilibria, chemical equilibria, and kinetics and use them to make predictions
- Demonstrate that statistical mechanics bridges the gap between quantum mechanics and classical physics
- Express the appropriate form of the partition function for a system
- Think creatively to solve problems

Textbook

Physical Chemistry: A Molecular Approach, by Donald A. McQuarrie and John D. Simon, ISBN: 978-0-935702-99-6.

Grade

Homework (approximately weekly):	25%
Midterm Exam 1	22.5%
Midterm Exam 2	22.5%
Final Exam (cumulative)	30%
Extra Credit	10%

Active Learning Environment

This course will promote an active learning environment. Throughout the course, we will do some in-class problem solving. Everyone will be given a few minutes to solve a given problem on their own. After making an effort to solve the problem, you will have an opportunity to compare solutions with your neighbors and discuss different strategies for approaching the problem. We will then reconvene as a class to see which problem solving strategies worked best. From time to time, I may ask volunteer students to help explain a topic that others are struggling with. Sometimes hearing an explanation from a fellow student makes something easier to understand than hearing it from the instructor.

Exams

For each midterm exam, you will be allowed to prepare and use one 8.5" × 11" sheet of notes (front-side only). On the final exam, three pages will be allowed. In addition, you will be allowed to use a calculator on all exams. Please bring your own, as there will be no extras available at the exam. The midterm exams will not be cumulative, but the final exam will cover material from the entire course.

Problem Sets

Approximately ten problem sets with Thursday due dates will be assigned. Collaboration is encouraged; however, before collaborating with your classmates, you should make an honest and significant effort to work through each problem on your own, and the problem set solutions must be written-up individually. Do not copy or paraphrase anyone else's work without giving proper credit. The use of online homework solution services (e.g. Chegg) will be considered a violation of the Honor code.

Open Ended Problems (OEP)

Open ended problems are problems that don't provide a straightforward answer, and may be from fields other than chemistry. They may require you to find or estimate data and will require you to devise a method of finding a reasonable answer with correct units. These problems will be graded on whether the approach used to solve the problem is reasonable, not for finding the correct answer. As scientists, we are often faced with problems that we don't immediately know how to solve. The OEP will give you an opportunity to practice this kind of problem solving.

Extra Credit

Problem sets may contain one or more "extra credit" problems which are somewhat more difficult than the others. Extra credit points are explicitly off the curve to encourage collaborative problem solving on these problems. By doing these harder, optional problems, you can earn enough extra credit during the semester to increase your score by a full letter grade. No other extra credit will be given other than these optional problems.

Late Policy

Problem sets are due by 5:00 PM on Thursday. A problem set that is turned in before the following Wednesday at 5:00 PM will receive half-credit. Problem sets will not be accepted after 5:00 PM on the Wednesday following its original due date. In addition, each student will receive one "no questions asked" extension during the semester, whereby you may turn a problem set in by Monday at 5:00 PM for full-credit.

Honor Code

This class follows the binding Code of Honor at Notre Dame. The graded work you do in this class must be your own. In the case where you collaborate with other students, make sure

to fairly attribute their contribution to your assignment. The full Code and a Student Guide to the Academic Code of Honor are available at: http://honorcode.nd.edu/

Office of Disability Services Statement

It is the policy and practice of The University of Notre Dame to provide reasonable accommodations for students with properly documented disabilities. Students who have questions about the Office of Disability Services or who have, or think they may have, a disability are invited to contact the Office of Disability Services for a confidential discussion in the Sara Bea Learning Center for Students with Disabilities or by phone at (574) 631–7157. Because the University's Academic Accommodations Processes generally require students to request accommodations well in advance of the dates when they are needed, students who believe they may need an accommodation for this course are encouraged to contact the Office of Disability Services at their earliest opportunity. Additional information about Disability Services and the process for requesting accommodations can be found at http://disabilityservices.nd.edu.

Calendar

Date	Topic	Assignment	Due Today
T 01/21	Syllabus & Overview		
Th 01/23	Entropy	Problem Set 1	
T 01/28	Entropy		
Th 01/30	Probability Distributions, Thermodynamic Terms	Problem Set 2	Problem Set 1
T 02/04	Ensembles & Partition Functions		
Th 02/06	More Partition Functions	Problem Set 3	Problem Set 2
T 02/11	Deriving Partition Functions and Collective Properties & Diatomics		
Th 02/13	Rotations & Level Populations	OEP 1	Problem Set 3
T 02/18	Polyatomic Molecules		
Th 02/20	**Exam 1**		
T 02/25	State Variables/State Functions/Heat/Work		
Th 02/27	Processes and Pathways	Problem Set 4	OEP 1
T 03/04	Thermodynamic Cycles		
Th 03/06	Laboratory Conditions and Free Energy	Problem Set 5	Problem Set 4
T 03/11	*Midterm Break—No Class*		
Th 03/13	*Midterm Break—No Class*		
T 03/18	*No Class*		
Th 03/20	Enthalpy/Gibbs Free Energy	Problem Set 6	Problem Set 5
T 03/25	Maxwell's Relations		
Th 03/27	Thermodynamics of Rubber Bands, Mixtures, Vapor Pressure	OEP 2	Problem Set 6
T 04/01	Phase Equilibria		
Th 04/03	**Exam 2**		

Date	Topic	Assignment	Due Today
T 04/08	Connecting Chemical Equilibria to Statistical Mechanics		
Th 04/10	Basics of Kinetic Theory of Gases	Problem Set 7	OEP 2
T 04/15	Kinetics, Collision Theory, and Rate Laws		
Th 04/17	Elementary Steps, Approximations, and Reactions	Problem Set 8	Problem Set 7
T 04/22	Transition State Theory		
Th 04/24	A Few Last Kinetics Topics		
T 04/29	*Last Day of Class*–Wrap Up		Problem Set 8
T 05/06	**Final Exam**		