Course Information

This dry but (hopefully) useful handout contains basic information about the course, how it will be run, when and where things will happen, grading policy, etc. Barring unforeseeable disasters or administrative whims (giving rise to remarkably predictable disasters), this information should not change. However, I will keep you informed should any changes occur.

Basic Information

This is a course in physical chemistry focusing on statistical mechanics, thermodynamics, and kinetics. It is assumed that you have completed the listed pre-requisites. If not, please see me as soon as possible.

The text for the course is *Thermodynamics, Statistical Mechanics, and Kinetics* by Andrew Cooksy. This book is required. Note that this is a change from the book used in the Quantum Mechanics and Spectroscopy course!

Lectures are scheduled to meet from 9:30 - 10:45 am Tuesdays and Thursdays in room L120 of the 12 Waverly Place building. In addition to the lecture periods, all students must sign up for one of the three recitation sections. These will be held on Mondays from 11:00 am to 12:15 pm in room 207 of the 194 Mercer Street building and from 12:30 am to 1:45 pm in room 209 of the 194 Mercer Street building.

Midterm exam date: There will be one midterm that will take place during the class period on Thursday, November 6.

Final exam date: Tuesday, December 16 from 8:00 am to 9:50 am. Location to be announced.

General goals and philosophy of the course

Both sections of physical chemistry (Quantum Mechanics and Spectroscopy; Thermodynamics and Kinetics) are and will be unlike any other chemistry course you have taken thus far (with the exception of those students who sweated through my Honors General Chemistry course!). Physical chemistry is that subdiscipline of chemistry that seeks to describe chemical systems, including individual molecules, gases, liquids, solids, solutions, etc. in terms of basic physical principles. Why is such a course required for chemists? Chemistry is a field that is grounded in the basic principles of physics, and therefore, physical chemistry is the most fundamental of all the subfields of chemistry. Other areas such as organic chemistry, inorganic chemistry, materials chemistry, nanoscience, medicinal chemistry, biochemistry,... are built upon the foundation of physical chemistry. You cannot fully understand the structure of an organic molecule, for example, without first understand what a chemical bond is. In order to understand the chemical bond, you need to understand quantum theory, which is one of the cornerstones of modern physics. You cannot understand biochemical reactions without first understanding thermodynamics, kinetics, and even some statistical mechanics. Our goal, therefore, in the two semesters you will spend learning physical chemistry is to give you a solid foundation in the physical principles and concepts you will need to understand other areas of chemistry. Because physical chemistry has a strong mathematical component, many of you will have put off this course as long as possible,
which means that you will need to apply some backward thinking to the courses you have already taken in order to gain this level of understanding. However, for those of you who plan to continue studying chemistry or a related field, you should find that the physical insights you gain here will give you a fresh perspective on the topics you will study in the future.

**Course content in brief**

This course will cover Chapters 1, 2, 4, 5, and 7-14 of the text (see course syllabus for details).

In addition to the aforementioned book chapters, I want to make clear at the outset that the material in the book is a *subset* of what we will cover in the course. This means that we will also delve into topics that you will not find in the book. Supplementary topics are intended to give you a more modern and broad perspective. Much of this supplementary material will come from current research and has been selected to clue you in to some of the most recent exciting discoveries and newest methods in modern chemistry. Generally, everything we cover in class can be found in the lecture notes on the course Web page (see below).

**The role of math and physics in the course**

Chemistry, like physics, is a quantitative science rather than a descriptive one. Answers in chemistry are expressed as real numbers corresponding to observable properties of a system. In order to arrive at such numbers, you must be capable of translating a complicated situation into the appropriate mathematical language and then applying mathematical methods to solve the resulting equations. It should be clear, then, that mathematics is the underlying language of the quantitative sciences, and in order to use it, you must be reasonably fluent in its vocabulary.

As you look through it, you will discover that the book assumes you have a working knowledge of functions of several variables, partial differentiation, multi-dimensional integration, vectors, and simple differential equations. It is assumed that you either have previously encountered these topics or are learning them concurrently. If this is not the case, you should speak to me as soon as possible. All of these topics will be used in lecture and will be needed for exams and homework assignments. Math is an integral (no pun intended) part of science and will therefore figure prominently in the course. In order to help you review, if you feel you need it, I have posted a “Mathematical Preliminaries” document on the course Web page (see below). I strongly recommend that you study it and make sure you are clear on all of the concepts in it. In addition, you should carefully study Chapter A of the textbook. If anything is unfamiliar to you, or even if you have questions about a topic you thought you understood well, do not hesitate to come to office hours to discuss it with me.

It is also assumed that you have some prior knowledge of basic physics. Given that this is a physical chemistry course, our focus will be on the physical principles that underly the chemical concepts we will discuss. This interdisciplinary approach will introduce you to a trend that is becoming more and more prevalent in science, namely, that the boundaries between the traditional disciplines, e.g. physics, chemistry and biology, are becoming blurred as researchers refocus their efforts in fields such as materials design, nanoscience, rational drug design, proteomics, etc. which require knowledge of several of the traditional disciplines.

**Teaching assistants and faculty fellow**

Your teaching assistant (TA) for the course are Peng Gao, who is a graduate student in the department of chemistry. He will be in charge of the two recitation sections. Although I will be working together with the TA throughout the course, the person ultimately responsible for the content of the course and the grading is me. Therefore, please do **NOT** go badgering the TA about issues/concerns that you should be discussing with me.

**My coordinates, office hours, and all that**
My office is located in Room 1001L Silver. I will hold regularly scheduled office hours each week at a time to be agreed upon by the class based on availability. During scheduled office hours, you are welcome to show up whenever you like. If you cannot make it to office hours or need to see me at another time for some reason, I will be happy to set up an appointment with you, where I can give you my undivided attention. I am often in my office and generally like to maintain an open-door policy. You should not feel intimidated about coming during office hours, and I do not mind if you drop by outside of office hours. I enjoy interacting with new students and want to get to know you better. However, just keep in mind that outside of office hours, there is a good chance that I will not be immediately available and that you might have to wait to have your question answered. Apart from teaching this class, I run a full-time research group and have numerous research projects of my own. Thus, you will often find me talking with one of my graduate students or postdocs, analyzing data myself, or preparing a grant proposal. This does not mean that I do not take undergraduate teaching seriously. In fact, part of what makes research-active professors effective teachers is the emphasis they place on research.

You can always reach me by e-mail if you need to. I will be happy to answer your questions or set up appointments this way. If I don’t respond to your e-mail right away, it either means that I am out of town (which is often the case) or simply unable to respond to your inquiry at that moment. Be patient! I will get back to you as soon as I am able do so.

There is a web page for the course. The URL is:

http://www.nyu.edu/classes/tuckerman/pchem

This course introduction will be posted there as well as lecture notes, interesting links, and who knows what else. This is a new page and is continually under construction, so you log onto it often.

We will also be making use of the online system, NYU Classes. The NYU Classes site can be accessed through your home.nyu.edu account by clicking on the “Academics” tab. You should see the link to the course there. If you do not have such an account, you can create one for yourself by going to http://start.nyu.edu

NYU Classes is an interactive forum for the course that contains discussion board and real-time chatrooms. Please RESTRICT YOUR USE OF THESE UTILITIES TO COURSE-RELATED DISCUSSIONS! I will be checking in often to make sure that posted questions are answered and that discussions do not go too far astray. I anticipate that NYU Classes will be a useful addition to the course, and I encourage everyone to take advantage of it. We will make use of its real-time discussion tools for exam review sessions.

**Grading**

The grading will be as follows: The midterm will count for 30% each, the final for another 30%, quizzes, 15% and homework 25%. The purpose of graded homework is to encourage you to do it. Science and math courses cannot be taken as “spectator sports.” The only way to learn the material is to solve problems. If you do find yourself falling behind, or having trouble with a homework assignment, exam, or quiz, contact me as soon as possible. Although I will already know that you are having trouble, the onus is on you to do something about it. I will do everything I can to help you catch up, address specific issues, or clear up any misunderstandings.

**Homework and quizzes**

Homework will be divided into two parts. For each chapter, I will assign a small number of problems from the book. These should be regarded as practice problems, by which you can gauge how well you have understood the basic concepts covered in that chapter. Although you will be required to turn these in, they will not be
graded. I will simply check to see that you have done them. In total, these practice problems will count for 5% of the 25% homework grade. This means that you will receive full credit simply for doing them.

Then, for each chapter, there will be a separate set of typically 3-5 problems designed to make you think more deeply about the material and to stretch you beyond just the basic concepts. These must also be turned in and will be graded. In total, these separate problem sets will count for the remaining 20% of the 25% homework grade. I encourage you to work together on these more difficult problems. Form study groups and discuss the problems together. Even if you feel that you have mastered the problems, you will benefit by having to explaining your ideas and your solutions to others. Working in groups, however, should not be a substitute for thinking about the problems independently, and everyone is expected to turn in their own work. Copying someone else’s work is not only plagiarism (see below) but will only hurt you when you are finally asked to demonstrate your problem-solving skills on exams. After the problem sets have been turned in, I will post the solutions online. Problem sets will generally be given out on Thursdays and due one week later at class, but, I will specify the due date with each assignment. No late homeworks will be accepted!

According to this schedule, recitations will focus on going over the problem set just handed in. There will be roughly one quiz per week given in recitation. They may be less frequent than this. In any case, they will be announced one or two days before they are given. Quizzes will be of a more straightforward nature, on the level of the practice problems, mainly so that I can monitor your basic mastery of the material.

Lecture/recitation attendance, missed exams, and other unpleasanties

Although attendance will not be taken at lectures or recitations, by not attending, you run the risk of missing material that cannot be found in the book. As a reminder, lectures will not simply be recapitulations of the book. Remember that the book is only a subset of the course material. In addition, I look at things quite differently from the authors and will present an alternative perspective as well as supplementary material. Also, numerous visual demonstrations based on computer simulations from actual research problems will be presented. Therefore, I encourage you to attend both lectures and recitation sections.

On a more grim note, there is no makeup for the midterm exam. Students who miss the midterm for a valid, documented reason will have the exam dropped from their final grade, and the final will count for a full 60% of your grade. Students who miss the midterm and who do not have a valid, documented excuse will receive a 0 for the midterm, and this will be averaged into your final grade for the class. Standard CAS policy is to allow a makeup final exam for students with documented proof of serious illness only. Students who manage to miss both the midterm and the final will fail the course. Under certain very limited circumstances, I will allow quizzes to be made up. Again, a valid, documented excuse must be presented. A quiz can only be made up within 1 week of the original date of the quiz. Keep in mind, however, that you are then at my mercy for scheduling the make-up quiz, and there is no guarantee that I will be able to fit you into my incredibly busy schedule this semester, so you run a risk by missing a quiz. Students who fail to make up a quiz within the one-week time frame will receive a 0 for the missed quiz.

If you experience medical problems during the term or if, for some other valid reason, must miss a number of lectures, please come and talk to me as soon as you can. Often something can be worked out.
Cheating

Cheating is a **SERIOUS** issue. This includes any form of plagiarism, copying, or collusion during quizzes, the midterm or the final. Anyone caught cheating will be severely punished. It is your responsibility to avoid any hint of cheating.

It is an unfortunate fact that students cheat in college and sometimes get away with it. This department is particularly adept at catching cheaters. If you are caught cheating, you can expect:

1. an F in the course,
2. to be brought up on charges before the Dean of the College,
3. possibly to be thrown out of school with a notation on your record as to why.

In case you do not fully comprehend what this means, a notation on your record means no medical school, no graduate school and, quite possibly, severe difficulties finding a job.

Reread the above before you consider cheating.

There is never a good excuse for cheating. If you find you are having difficulties, come talk to me. If you feel that you cannot do that, go to the Student Services section of the CAS Dean’s Office on the 9th floor of Main.

---

**Getting the most out of the course**

Work together! It is quite possible to do very well on your own, but collaborative efforts often make greater breakthroughs. Not only can you learn from someone else and how they think about the material, but also answering someone’s questions helps you arrange the material logically on your own mind. Come to lectures, and keep in mind that the TA and I are here to help you learn. Clearly, we cannot do this for you, but we can make it easier. Work hard and come talk to us when you need. Ultimately, we want everyone to do very well, enjoy the course, and get something out of it, for then we know that we have done our job.
Syllabus

I. **Week 1**

1. 9/2/2014:

2. 9/4/2014:
   - *Problem set 1 given out.*

II. **Week 2**

1. 9/8/2014:
   - *Quiz 1 given at recitation.*

2. 9/9/2014:

3. 9/11/2014:
   - *Lecture 4*: Van der Waals coefficients.
   - *Problem set 1 due.*
   - *Problem set 2 given out.*

III. **Week 3**

1. 9/15/2014:
   - *Quiz 2 given at recitation.*

2. 9/16/2014:
   - *Lecture 5*: Pair correlation functions.

3. 9/18/2014:
   - *Problem set 2 due.*
   - *Problem set 3 given out.*

IV. **Week 4**

1. 9/22/2014:
   - *Quiz 3 given at recitation.*

2. 9/23/2014:
   - *Lecture 7*: Mass transport (finish), computers in statistical mechanics (beginning)
3. 9/25/2014:
   * Lecture 8: Computers in statistical mechanics (continue)
   * Problem set 3 due.
   * Problem set 4 given out.

V. Week 5
1. 9/29/2014:
   * Quiz 4 given at recitation.

2. 9/30/2014:
   * Lecture 9: Computers in statistical mechanics (finish).

3. 10/2/2014:
   * Lecture 10: First law of thermodynamics and heat capacities.
   * Problem set 4 due.
   * Problem set 5 given out.

VI. Week 6
1. 10/6/2014:
   * Quiz 5 given at recitation.

2. 10/7/2014:
   * Lecture 11: First law of thermodynamics, Legendre transforms, and free energies.

3. 10/9/2014:
   * Lecture 12: Second and third laws of thermodynamics (beginning)
   * Problem set 5 due.
   * Problem set 6 given out.

VII. Week 7
1. 10/13/2014: Fall recess, no quiz.
2. 10/14/2014: Fall recess, no class.
3. 10/16/2014:
   * Lecture 13: Second and third laws of thermodynamics (beginning)
   * Problem set 6 due.
   * Problem set 7 given out.

VIII. Week 8
1. 10/20/2014:
   * Quiz 6 given at recitation.

2. 10/21/2014:
* Lecture 14: Theory of phase transitions (beginning)

3. 10/23/2014:
   * Lecture 15: Theory of phase transitions (finish)
   * Problem set 7 due.
   * Problem set 8 given out.

IX. Week 9
1. 10/27/2014:
   * Quiz 7 given at recitation.

2. 10/28/2014:
   * Lecture 16: Solutions (beginning)

3. 10/30/2014:
   * Lecture 17: Solutions (finish)
   * Problem set 8 due.
   * Begin midterm review – no problem set.

X. Week 10
1. 11/3/2014:
   * Midterm review. No quiz.

2. 11/4/2014:
   * Lecture 18: Thermochemistry.

3. 11/6/2014:
   * Midterm on chapters 1, 2, 4, 6-9
   * Problem set 9 given out.

XI. Week 11
1. 11/10/2014:
   * Quiz 8 given at recitation.

2. 11/11/2014:
   * Lecture 19: Chemical equilibrium

3. 11/13/2014:
   * Lecture 20: Introduction to reaction kinetics – rate laws (beginning)
   * Problem set 9 due.
   * Problem set 10 given out.

XII. Week 12
1. 11/17/2014:
* Quiz 9 given at recitation.

2. 11/18/2014:
   * Lecture 21: Introduction to reaction kinetics – rate laws (finish)

3. 11/20/2014:
   * Lecture 22: Reaction mechanisms I – complex reaction mechanisms.
   * Problem set 10 due.

XIII. Week 13

1. 11/24/2014:
   * Quiz 10 given at recitation.

2. 11/25/2014:
   * Lecture 23: Reaction mechanisms II - Steady-state and equilibrium approximations.


XIV. Week 14

1. 12/1/2014:
   * Quiz 11 given at recitation.

2. 12/2/2014:
   * Lecture 24: Enzymatic reactions and Michaelis Menten kinetics.

3. 12/4/2014:
   * Lecture 25: Reactor design I - batch and constantly-stirred tank reactors.
   * Problem set 11 given out.

XV. Week 15

1. 12/8/2014:
   * Quiz 12 given at recitation.

2. 12/9/2014:
   * Lecture 26: Reactor design II - plug flow reactors.

3. 12/11/2014:
   * Lecture 27: Catalytic reactions.
   * Problem set 11 due.

XVI. Week 16

1. 12/16/2014: Final exam from 8:00 am to 9:50 am.