CHEM 342

Physical Chemistry II

Spring 2023

INSTRUCTOR

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OFFICE HOURS

MWF: 9:15 – 10:55 AM or by appointment

LECTURES

MWF: 11:00 – 11:50 am, 153 Roddy Hall

LABORATORY

Section A Tuesday: 1:10 – 4:00 pm, 226 Caputo Hall

TEXTBOOK

Physical Chemistry, 3rd edition, by Thomas Engel & Philip Reid, Pearson/Benjamin Cummings, 2013; ISBN: 032181200X

SUPPLEMENTAL MATERIAL

Required for exams and homework: A calculator with root, logs and antilogs will be requried for exams. Some cheap calculators that work well are the Casio FX250HC, the Sharp 501WBBL, and the Texas Instruments TI30X. All these calculators, and many others appropriate for this course, are available for less than ten dollars. You will need to purchase a bound lab notebook for recording your observations during lab. (You may use the same notebook you used in CHEM 341 if there are sufficient blank pages.) You must provide your own safety glasses and wear them at all times while you are in the laboratory, along with covered-toe shoes. Additionally, a computer with word processing software such as Microsoft Word, and spreadsheet functionality such as Microsoft Excel, will be useful for writing lab reports.

COURSE PREREQUISITES

Prior to enrolling in physical chemistry, the student should have successfully completed two semesters of general chemistry, two semesters of calculus-based general physics, three semesters of calculus, one semester of quantitative analysis, and one semester of the fundamentals of writing. According to the undergraduate catalog, the prerequisite course for CHEM 342 is CHEM 341, and the prerequisite courses to CHEM 341 are CHEM 265, PHYS 232, MATH 311 and ENGL 110.

COURSE CONTENT

Physical Chemistry II covers, broadly, three areas: ***chemical kinetics*** (the rates of chemical reactions), an introduction to ***quantum mechanics*** (the mathematical framework for predicting the behaviors of microscopic particles) and applications of quantum mechanics to problems of chemical interest, and ***spectroscopy*** (the study of the interaction of radiation with matter). The course content is taken from the textbook along with occasional supplementary material available on D2L.

PHYSICAL CHEMISTRY: AN INTRODUCTION

What is physical chemistry?

Physical chemistry is the application of the principles and methods of physics and mathematics to chemistry. Physical chemistry can also be regarded as the study of the physical principles underlying chemistry. We want to know how and why materials behave as they do. The ultimate goal of physical chemistry is to provide a (mathematical) model for all of chemistry.

What level of mathematics is required?

The champion of Copernican heliocentrism, Galileo, made great contributions to physics even without knowing algebra, which had been invented by the Arabs but did not come into general use in Europe until the late seventeenth century. He relied on dialogues and on the geometry of the Greeks to communicate his ideas to his contemporaries. Imagine how difficult it was for him to to explain physical laws without using algebra! Physical chemistry concepts solicit a mathematical framework for their presentation as well, and they require that calculus be used as a tool just as algebra has been used as a tool in previous courses. In the same way that algebra facilitated the study of actions under constant forces, calculus facilitates the study of actions under dynamic forces. The derivations and calculations of physical chemistry require many partial derivatives. (This is because we will need to algebraically manipulate functions of several variables.) Initially the functions and are mostly in one variable. Eventually there will be more functions in two and three dimensions. We will also perform a number of simple integrals in the set of real numbers. In the spring semester we will perform more integrals in the domain of the set of complex numbers.

PHYSICAL CHEMISTRY COURSES AT MILLERSVILLE UNIVERSITY

At Millersville University the two regular semesters of physical chemistry for chemistry majors are numbered CHEM 341 and CHEM 342. The general outline of coverage for each semester is:

CHEM 341

- Chemical thermodynamics (thermodynamics applied to chemistry problems)
- Introduction to statistics and combinatorics, as time permits
- Equilibrium statistical thermodynamics, as time permits

CHEM 342

- Introduction to quantum mechanics (applied to problems of chemical interest)
- Spectroscopy (the interaction of radiation with matter)
- Chemical kinetics (study of the rates of chemical reactions)

Thermodynamics is usually called a ***macroscopic*** theory. That is, it deals with the bulk properties of matter and does not concern itself with whether or not atoms or molecules even exist. On the other hand, quantum mechanics is a ***microscopic*** theory because it deals with the individual particles of matter and light. Statistical thermodynamics brings us full circle by providing a mechanism for calculating the properties of bulk material (macroscopic samples) from the properties of the atoms and molecules which comprise the material. Much recent interest has developed in the so-called mesoscopic materials, which are composed of relatively small numbers of particles. They consist of so few particles that they do not manifest the same properties as the bulk matter, yet they have enough particles that they no longer have the properties of individual atoms or molecules. Work in this area has given rise to various "nanoscale" technologies.

COURSE OBJECTIVES

1. The student will demonstrate an understanding of the principles, laws and theories of physical chemistry.
2. The student will develop the ability to solve quantitative problems.
3. The course will promote original thought on the part of the student and encourage the use of logic in the solution of problems.
4. The student will develop an ability to learn and work independently.
5. The student will apply the skills learned in general chemistry, general physics, and differential & integral calculus to chemical problems.
6. The course will introduce the Dirac notation and other notation useful for communicating quantum mechanical problems of chemical interest.
7. The course will provide the student with an opportunity to perform quantitative empirical studies in the laboratory.
8. The student will develop their abilities for communicating, in written form, the results of the experiments.

EXAMINATIONS

Tentative Lecture Exam Schedule:

Exam 1: Friday, Feb 10 (Chapters 33 – 36)
Exam 2: Friday, Mar 17 (Chapters 12 – 17)
Exam 3: Friday, Apr 7 (Chapters 18 – 20)
Exam 4: Wednesday, April 28 (Chapters 21 – 27)
Final Exam (Comprehensive): Thursday, May 4, 8:00 am

All examinations will count toward the course grade and it is expected that students will complete all of the examinations at their regularly scheduled times.

Suggested problem sets will be assigned via Desire2Learn, but they will not collected, or graded if submitted. Their completion is optional, but you are advised to attempt at least one of each type of problem as preparation for the examinations. We will have time in class, or outside of class at a mutually agreeable time, to work some problems after you have made an attempt to work them yourself. For updates, please visit the D2L website at https://millersville.desire2learn.com/

ON-LINE COMPONENTS

Posted on the Desire2Learn website you will find various assessment tools and discussions, as well as links to external websites. Please note the due dates for these components. *Late submissions will not be accepted under any circumstances.*

GRADING

Grading will be as follows, but the instructor reserves the right to shift the curve in favor of a higher number of students making higher letter grades. It is possible that everyone in this class will earn an A. It is possible that everyone will earn an F. I expect that this generally will not happen. The total possible points are as follows:

Exam 1	100	Lecture: 750 points
Exam 2	100	
Exam 3	100	
Exam 4	100	
On-line components	150	
Final exam	200	
Lab reports (4)	160	Lab: 250 points
Notebook, S&P	50	
Proposed Lab Video	40	
Total	**1000 points**	

900 points guarantees at least an A-
800 points guarantees at least a B-
700 points guarantees at least a C-
600 points guarantees at least a D-

LAB CONTENT

Physical Chemistry laboratory provides the student a chance to develop techniques in making physical measurements. Our laboratory is meant to simulate scientific investigation, but is limited by the amount of time that one can spend on a given topic, and limited also by the fact that truly ***new*** scientific discoveries are not likely within our course. What we attempt to do here is bridge the gap between our sterile, lecture-based knowledge of the details of the workings of the Universe, and the actual Universe, as perceived by ‘first-person’ observation. You are familiar with direct observation, and you are familiar with the concepts of Chemistry. Now, you are challenged to make an observation that quantitatively demonstrates a rigorous concept that you have been taught, but make this concept meaningful for you through personal experimental experience. No one wants to be a pre-programmed machine, nor do I wish to create one in you. The protocols for each experiment are meant to guide you through your observations, and are not to be treated as a list of commands to be executed. On the other hand, if you went into the laboratory without any instructions at all, it would take you too long to get the equipment working, and this detracts from the experience of persuading nature to reveal her secrets.

Treat this course as yours. When you are in physical chemistry lab it is your own chemistry laboratory. Be ready to take instruction and criticism like you have in many other courses, but be ready to learn creatively, with instruments that extend your innate senses. Scoutmasters famously utter the scouting motto: *Be prepared.* This is a fitting motto for scientific lab courses as well. If you have not thought through what you are about to do in the lab, you will not be able to observe anything except confusion. Read the lab protocol well before the lab is to occur and ruminate on the experience to come. Reread the instructions and predict for yourself what might occur in the lab.

RECORD-KEEPING IN THE LABORATORY

To properly apply the scientific method, you must record all laboratory observations with *ink* in a bound notebook in great and graphic detail (pretend you are Leonardo da Vinci; mirror script is optional). Also, bear in mind that the lab notebook is a legal document that is regarded as the *primary source* of data, and it can be crucial in disputes over patent claims or first discovery. The notebook should have a table of contents at the beginning, containing the experiment title, the page on which each experiment begins, and the date(s) during which the experiment was performed. The pages should be numbered, and no pages should ever be removed from the notebook. At the beginning of a new experiment in the notebook, write a few sentences about the purpose of the experiment, the method used, where the procedure can be found, and any partners with whom you will work. Mistakes are indicated by a single line drawn through them, never by obliterating them beyond recognition, since experimenters often decide later that what was thought to be a mistake was not really a mistake.

Observations and data should be recorded directly into the notebook *as you are doing the experiment*. Do not write on paper towels or scrap paper and transfer to the notebook later. This defeats the purpose of the notebook as a primary data source. You should organize your notebook beforehand when possible by labeling and leaving blanks for experimental parameters that must be recorded, and by making tables for data ahead of time. If you are unsure whether a piece of information should go into the notebook, write it in there. You can never have too much information. If you have misgivings about the accuracy or precision of the data, or if something went wrong during the experiment, write that in the notebook as well. Later, you won't remember which data you trust and which you do not. Explanatory notes, units and labels are always important, as is legibility.

Experimenters sometimes work alone but more often work in small teams. You will be divided into teams of two or three people. The teammates that you have in this class are there to share ideas, data, and effort, but not papers. Each of you must ultimately compile your work individually into something that is publishable. This is how real labs work, and your university laboratory experience should emulate real-world laboratory experience. An experiment is not complete until the results are analyzed and the conclusions are presented in an original composition. You will write about each experiment as if it were original work without exact precedent. (Feel free to have fun with this anachronistic concept). The form, length and style are to be that consistent with papers to be submitted for publication in the peer-reviewed journals. See the Lab Report Style Guide posted on the elearning website. Also, take a look at the reports in *Chemical Physics Letters* or the *Journal of Physical Chemistry* or the *Journal of*

Chemical Physics. You will need to peruse these journals in the library for examples and the instructions to authors. You need only write lab reports for four of the experiments performed. I will let you know which four in class or on Desire2Learn.

EXPERIMENTS

The experiments for the course are listed below, along with experiment number from the lab manual. A full report should be written for four of these experiments. A style guide for lab reports will be posted on the Desire2Learn website. Due dates will be announced in class or on Desire2Learn. *Late penalties for lab reports will be severe, with a minimum 25% penalty.*

Tentative list of experiments	**filename on D2L**
Kinetics A: Rate Constants and Activation Energy	kinetics or EsterHydrol
Surface Tension of solutions	ST (capillary or DuNouy)
Eutectic Point Determination	eutectic
IR & Raman Spectroscopy of Dichlorobenzenes	RamanIR & Spartanvideo
Line Spectra & Bragg's Law	spectra
Absorption Spectrum of Conjugated Dyes	dyes
Fluorescence spectroscopy	Fluorescein
Rotation-Vibration Spectrum of HCl & DCl	HCl instructions

TENTATIVE LAB SCHEDULE

First week: Introductions, overview, safety, analysis, proper presentation of data and results, and scheduling.

Beginning on the second week we will follow a rotating schedule. See the schedule posted on D2L for details.

Laboratory report due dates will be posted on in the lab schedule on D2L.

PROPOSED LABORATORY EXERCISE

In addition to the four typed reports over experiments you have performed, you will propose a laboratory experiment in the form of a short video. This experiment should be original and use available equipment. It can be the same as your fall proposal. The criterion used in evaluating a proposed experiment is whether it should be attempted next semester as a possible replacement or alternative for a current experiment. You should request approval of your idea for a proposed experiment before submitting the video. For assistance in making videos or to borrow recording equipment, contact the Digital Learning Studio, which has offices in Stayer Hall and in the McNairy Library. The due date for this video is 5:00 pm on the same day as your final exam.

ATTENDANCE

Concepts are cumulative in the sense that the student must master introductory concepts and derivations in order to fully understand more advanced topics in physical chemistry. We will continue to build on our earlier understanding. Because of the mathematical nature of physical chemistry, attendance is required for this course. If you cannot attend class, due to illness or other emergency, you should contact me before the class period, or as soon thereafter as possible. Poor attendance will affect your class grade. You will find this applies to most of your upper-division coursework. You should also note the last day to drop under Important Dates.

DISABILITY STATEMENT

It is the responsibility of students who have professionally diagnosed disabilities to notify the instructor so that appropriate modifications can be made to meet any special learning needs. Specific questions regarding accommodations for students with disabilities should be directed to Student Learning Services, located in Room 352 of Lyle Hall, or send an email to Learning.Services@millersville.edu

ACADEMIC DISHONESTY

Academic dishonesty includes unfairly advancing one's own academic performance or the performance of another, as well as intentionally limiting the academic performance of another student. *Do not plagiarize each other's lab reports.* Your university's accreditation is based, in part, on academic standards of excellence. Fraudulence and plagiarism will devalue your MU degree. Penalties for academic dishonesty will depend on the situation, ranging from a zero grade for the exam or assignment, to course failure. I hope this does not arise in this course.

IMPORTANT DATES*

January 17 – Day and evening classes begin
January 24 – Last day to drop or add a course online
January 24 – Last day to drop a course without a W
February 16 – Application deadline for spring degree
March 6 – Registration TAP available
March 6-10 – Spring Break, no classes
March 26-30 – ACS National Meeting
March 31 – Last day to drop/change course with a W
May 1 – Last day of regular class meetings for spring
May 4 – Final Exam, Thursday 8:00 – 10:00 am
May 6 – Spring 2023 Commencement

**Dates compiled from the current bulletin edition may change. It is the student's responsibility to remain apprised of all important dates.*